Mars Manual

ES3

August 3, 2012

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1 Introduction

MARS is a powerful and robust object-oriented solver for simulating the mechanical response of structural systems subjected to short duration events. It employs an explicit time integration scheme for solving the equation of motion of large systems. It implements all the capabilities and versatility of general finite element codes. In addition, MARS features some unique techniques, such as the Lattice Discrete Particle Model (LDPM) and adaptive remeshing algorithms for shell and solid meshes, which facilitate the solution of problems involving structural break-ups, fragmentation and post-failure response under extreme loading conditions.

MARS includes standard finite element and discrete element features such as:

- QPH quadrilateral shell elements with physical hourglass stabilization,
- DKT triangular shell elements,
- Beam elements with various built-in cross sections
- 8-Node Flanagan-Belytschko hexahedral elements with hourglass stabilization
- Hyper-elastic solid elements,
- Various constraint formulations, including concrete-rebar interaction, interaction,
- Automatic contact algorithm for node-face, edge-edge, node-edge, node-node contact detection,
- Macro-particles for simulating discrete elements with complex shapes.

Additionally, MARS has an object-oriented architecture, which makes it possible to add new capabilities in an efficient and systematic fashion. All entities in MARS are organized in a hierarchical framework. Classes of simple entities, such as edges and faces, are used to derive more complex entities, such as beams and shells. Since February 2011, MARS incorporates an interface which makes it possible for users to develop custom objects, element formulations, and lists. A user can derive new classes from existing ones and then modify them by inserting new features. For example, a Cosserat 10 node tetrahedral element was recently developed by a student starting from the already available 10-node tetrahedral element. The interface is very flexible and allows to incorporate any number of new objects (material models, special load histories, etc.) and lists (lists typically implement element formulations, interaction mechanisms, etc.).

MARS has been successfully adopted for the simulation of a wide variety of problems, which include:

- Modeling of cracking and failure of cement-based materials materials
- Response of reinforced concrete structures to blast loads and fragment impacts
- Cable dynamics problems
- Fragmentation of ordinance casings
- Laceration of plates and shells

1.1 The Lattice Discrete Particle Model (LDPM)

The Lattice Discrete Particle Model (LDPM), is a discrete meso-mechanical model for concrete, which was recently developed by Dr. Cusatis and co-workers at Rensselaer in collaboration with Dr. Pelessone at ES3. LDPM simulates the mesostructure of concrete by a three-dimensional assemblage of discrete particles whose position within the volume of interest is generated randomly according to the given aggregate size distribution. A whole section of this report is dedicated to LDPM.

LDPM has been extensively calibrated and validated in the last few years and it has shown superior capabilities in reproducing and predicting qualitative and quantitative concrete behavior under a wide range of loading conditions.

1.2 Fragmentation of Weapon Casings

The MARS fragmentation algorithm for solids inserts discrete cracks within a hexahedral mesh treating failure at the structural level rather than in the material constitutive equations. The initial mesh is subdivided into clusters of elements. Cracks may form between clusters when a local measure of damage exceeds a local allowable. Cracks can propagate and/or coalesce forming fragments of various shapes and sizes. The parameters of the algorithm have been calibrated for specific weapons so that generated fragment distributions match arena test data. data.

1.3 Nano-Scale Modeling of C-S-H

The discrete element capabilities of MARS were used to simulate the behavior of Calcium-Silicate-Hydrate (C-S-H) through nano-scale models of C-S-H specimens subjected to nano-indentation testing. The simulation results from these models are providing new knowledge in the nanomechanical behavior of C-S-H and are helping in formulating constitutive laws for higher scale simulations. simulations.

1.4 Parallelization

The MARS software can solve extremely large analytical models, which require extensive use of computer resources. The large demand on computer memory and CPU time can only be satisfied by using distributed-memory massively parallel computer systems, like the ones available at the ERDC supercomputer center. Over the last two years (2008-2010), MARS has been modified to implement domain decomposition and use the Message Passing Interface (MPI) protocol. This is an on-going area of research, which puts MARS at the leading edge of simulation software.

1.5 Vehicle Response to Blast

Conversion filters in MARS translate models developed for other codes. In the example below, the model of a Ford Taurus, developed at GWU for crash simulations, was employed to simulate the effect of surface charges applied on the vehicle.

1.6 Laceration of Plates and Shells

The MARS laceration algorithm is essentially a two-dimensional version of the solid fragmentation algorithm presented earlier. Cracks can develop between clusters of shell elements depending on specified local failure criteria. Cracks can propagate or coalesce to form tears. All material is fully accounted for as all mass is maintained and balanced.

1.7 Steel Plates Structures

Complex steel plate structures commonly found in civil and mechanical construction can be modeled in great detail with MARS. Contact conditions between all entities in the model ensure that plates do not penetrate each other. Rivet, bolt, or weld elements are used to hold plates and braces together.

2 Available Documentation

The MARS documentation consists of four different forms of documentation:

- An online manual hosted at http://www.es3inc.com/mechanics/MARS/Online/MarsManual.htm. This contains several examples with figures. However, since it is hosted at a remote web-site, that makes it difficult to keep it syncronized with the latest version

of MARS. As such, its use is more for general reference but not for specific instructions on how to use input commands.

- A blog hosted at http://es3-mars.blogspot.com/ . This is useful for providing a chronology of when new features are inserted in MARS.

- A built-in manual printed to an ASCII text file directly from the Mars executable. The information in the manual is consistent with the features built into the code. Indeed, it is relatively simple to update the documentation at the same time a new feature is added or and existing feature is modified, since documentation coexists in the same source files where the algorithms are implemented. implemented.

MARS is a fast developing solver, with new features being added on a regular basis and occasional reorganization of existing material. As such, the built-in ASCII manual was playing a critical role in providing updated documentation consistent with the version of the program from which it was printed. However, the format of the documentation was not practical, since it did not provide an updatable table of contents. Furthermore, it could only be explored using a text editor like vi or Notepad, which provide the basic 'find' tools for searching specific words inside a file. In February 2011, we realized that we could restructure the built-in manual and generate better quality documentation. Essentially, using the polymorphic properties of Object Oriented C-classes, we created three classes that would process the same information and generate three different types of documents:

- The ordinary ASCII text manual already available, obtained by executing Mars with the -H option (`mars -H`). Note that the name of the Mars executable may vary on different computer systems. Check section on computing platforms.

- An ASCII tex file which can be processed using LaTex for generating a pdf file with a hyperlinked table of contents. The LaTex file is generated using the `-Dl` option where `l` is the lower case letter l.

- A set of html files which can be accessed using any internet browser. Table of contents and hyperlinks are also available. These html files are generated in the current folder using the command `mars -Dh`. The files can be accessed with any web browser.

3 Code Architecture and Input Format

The MARS input decks consists of a sequence of blocks, called sections. Each section specifies the input for an entity, (e.g. material, load curve, etc.) or a list (finite elements of a component, external faces of a component, contact conditions, etc.). A special block referenced as `ControlParameters` includes run control commands and miscellanea information. The order in which these blocks of information appear in the MARS input deck provides some flexibility. The `ControlParameter` section must always be placed at the beginning of the input because it contains units selections. The definition of new

entities must be done before they are referenced in other parts of the input file. In this manual, we use the term 'entity' for individual objects, such as material models, reference systems, load curves, etc., and lists of objects, such as finite element lists, contact lists, constraint lists, etc.

Each entity is given a descriptive short name which is used as identifier in the rest of the input file and during post-processing. Similar entities must use unique names. However, the program does not preclude using the same name for dissimilar entities. For example, the list of external faces of a list of solid elements (solid component)can be given the same name as the name of the solid list. This is because a face list and a solid list are dissimilar.

A typical input file looks like this:

```
First line is always a title line
ControlParameters {
  . . .
}
Material Steel Elastic {
  . . .
}
NodeList PartNodes {
  . . .
}
//  Finite element definition
HexSolidList PartElements FBSingleIP {
  Material Steel
  Nodelist PartNodes
  . . .
}
//  Applied loads
LoadCurve NodalLoad {
  . . .
}
NodalLoadList Loads {
  Nodelist PartNodes
  LoadCurve NodalLoad
  . . .
}
//  Post-processing
TimeHistoryList History {
  . . .
}
PlotList Plot {
  . . .
}
EOF
```

3.1 Major Syntax Rules

The current MARS format adopts a syntax style which resembles the C++/Java styles with long descriptive keywords. Comments can be entered using the // characters at any place in a line (similar to the Fortran exclamation mark). Entire sections can be commented out using the '/*' sequence at the beginning and the '*/' sequence at the end. The C++ based syntax style makes it possible to take advantage of the vim (vi modified editor) syntax checker available on most Unix-based systems, including Linux. The vim syntax checkers paints words in a text file with different colors to differentiate number, comments, keywords, etc. The MARS syntax checker file is based on the C++ file with some modifications. modifications.

Each block of data is limited by curly brackets, as shown in the previous example. Within each block, there may be sub-blocks of data which are also contained in curly brakets. For example:

```
HexSolidList SolidPart FBSingleIP {
  NodeList Nodes
  EditNodeList {
    Move 2. in 0. in 0. in
  }
}
```

The commands inside these blocks are intended to be indented, with the number of spaces proportional to the level of indentation. Although MARS does not enforce indentation, it is good practise to consistently indent an input file; for example, indent by two spaces for each level of indentation. Indentation makes the input more readable.

3.2 The Solver Loop

The solver loop performs a sequence of tasks.

A summerized version of the solver loop is listed below. This is specially useful for those who intend to write user-defined objects and lists

```
    while (time < terminationTime) {
        // update MPI domains (if necessary)
        mpiDomains.update();
        // reset nodal forces and moments to zero
        for (jL = 0; jL < numLists; jL++)
            list[jL]->clearNodalForces();
        // compute nodal internal forces - apply external forces
        for (jL = 0; jL < numLists; jL++)
            list[jL]->calcFrc();
        // write time history output (if necessary)
        for (jL = 0; jL < numLists; jL++)
            list[jL]->writeTimHistRecord();
        // reduce forces for master-slave formulations
```

```
        // (node: loop uses inverse list order)
        for (jL = (numList-1); jL > -1; jL--)
            list[jL]->reduceFrc();
        // apply constraints
        for (jL = 0; jL < numLists; jL++)
            list[jL]->applyConstraints();
        // write 3-D plot file records (if necessary)
        for (jL = 0; jL < numLists; jL++)
            list[jL]->writePlotFile();
        // perform tasks from the action list
        for (j = 0; j < numActions; j++)
            action[j]->exec();
        // integrate equations of motion
        for (jL = 0; jL < numLists; jL++)
            list[jL]->integrateEOM();
        // apply kinematic conditions for master-slave formulations
        for (jL = 0; jL < numLists; jL++)
            list[jL]->applyKin();
        // update time parameters
        time += dt1;
        numSteps++;
        // go interactive if requested
        checkSignal();
    }
```

4 Control Parameters

The `ControlParameters` section follows the title line and is used for defining parameters that control the simulation or global parameters. The first command must always be the selection of units. A detail description of units is give in a separate subsection.

```
ControlParameters {
  // Unit specification should be the first input line
  Units English // more on this below
  TerminationTime  1. ms
  CurrentTime  0.1 ms
  MaximumTimeStep 0.001 ms
  TimeStepScalingFactor 0.8 // default 0.9
  FragmentationTimeInterval 0.005 ms
  / time or step cotrolled actions
  Monitor Frequency 10 // print progress line every 10 steps
  // more on this below
  PlottingDefaults { ... } // see below
  ContactDefaults { ... } // see below
```

```
  DynamicRelaxationCurve DynRelax
  NoDynamicRelaxation // stop dyn relax on restart
}
```

4.1 Unit Systems

The unit system to be employed in a simulation is specified using the command `Units` followed by one of the unit system label: SI / CGS / English / Nano.

1. SI: international, m, Kg, second
2. CGS: cm, gram, second
3. English: in, pound, second
4. Nano: nm, ng, ns

The unit system can be specified once, typically at the top of the `ControlParameters` section. All input quantities are converted to the selected unit system. For this reason, all quantities must be entered with their dimensional units. For example, if SI units are chosen and the user enters a time variable of 0.1 ms, this variable will be automatically converted to 0.0001 (s). This can be very useful for material properties; for example, the density of a material can be found in g/cm3 and it would be tricky for most analysts to convert it to the correct dimensions in English units. A list of available dimensional units is given in the next subsection.

4.1.1 Dimensional Units

Below is a list of implemented dimensional units and physical quantitities which are typically used for specifying input parameters of MARS structural models. This list is often updated with new quantitities and units depending on what new features are inserted in MARS. If the wrong units are used for an input parameter, MARS errors off and prints the available units from the list below.

The conventions described in "The Unified Code for Units of Measure" are employed. For SI and CGS systems, kilo (x 1,000) is denoted with the lower letter 'k' as in kg or km, Mega (x 1,000,000) with 'M', giga (x 1.e9) with 'G', milli (x 0.001) with 'm', micro (x 1.e-6) with 'u', pico (x 1.-9) with 'p'.

Quantity: Nondimensional

Reference unit: unit (no label necessary)
%:(0.01)

Quantity: Time

Reference unit: s
ms:(0.001) - micros:(1e-06) - s:(1e-06) - us:(1e-06) - ns:(1e-09) - mcs:(1e-06)

Quantity: Length

Reference unit: m
cm:(0.01) - mm:(0.001) - km:(1000) - in:(0.0254) - ft:(0.3048) - km:(1000) - nm:(1e-09) - mcm:(1e-06) - um:(1e-06)

Quantity: Area

Reference unit: m2
cm2:(0.0001) - mm2:(1e-06) - km2:(1e+06) - in2:(0.00064516) - ft2:(0.092903) - Km2:(1e+06) - nm2:(1e-18)

Quantity: Volume

Reference unit: m3
cm3:(1e-06) - mm3:(1e-09) - km3:(1e+09) - in3:(1.63871e-05) - ft3:(0.0283168) - km3:(1e+09) - nm3:(1e-27) - Km3:(1e+09)

Quantity: Mass

Reference unit: Kg
g:(0.001) - lb:(0.453592) - lb.s2/in:(175.127) - lb-s2/in:(175.127) - kg:(1) - ng:(1e-12) - nnKg:(1e-18) - mcg:(1e-09) - mg:(1e-06) - ug:(1e-09)

Quantity: Density

Reference unit: Kg/m3
g/cm3:(1000) - lb/in3:(27679.9) - lb.s2/in4:(1.06869e+07) - lb-s2/in4:(1.06869e+07) - lb/ft3:(16.0185) - kg/m3:(1) - nnKg/nm3:(1e+09)

Quantity: Velocity

Reference unit: m/s
cm/s:(0.01) - mm/s:(0.001) - Km/s:(1000) - in/s:(0.0254) - ft/s:(0.3048) - km/s:(1000) - nm/ns:(1) - Km/hr:(0.277778) - mph:(0.44704) - Knots:(0.514444)

Quantity: Force

Reference unit: N
dyn:(1e-05) - lb:(4.44822) - lbf:(4.44822) - kip:(4448.22) - nN:(1e-09)

Quantity: Pressure

Reference unit: Pa
psi:(6894.76) - ksi:(6.89476e+06) - lb-in-s:(6894.76) - MPa:(1e+06) - GPa:(1e+09) - dyn/cm2:(0.1) - nPa:(1e-09)

Quantity: Stress

Reference unit: Pa
psi:(6894.76) - ksi:(6.89476e+06) - lb-in-s:(6894.76) - MPa:(1e+06) - GPa:(1e+09) - dyn/cm2:(0.1) - nPa:(1e-09)

Quantity: Energy

Reference unit: J
erg:(1e-07) - ft-lbf:(1.356) - in-lbf:(0.113) - nJ:(1e-09) - nnJ:(1e-18)

Quantity: Stiffness

Reference unit: N/m
J/m2:(1) - dyn/cm:(0.001) - erg/cm2:(0.001) - lbf/in:(175.127) - nN/nm:(1)

Quantity: Rate

Reference unit: 1/s
1/ms:(1000) - 1/ns:(1e+09) - Hz:(1)

Quantity: Angle

Reference unit: deg
rad:(0.0174533)

Quantity: Momentum

Reference unit: Kg-m/s
Kg.m/s:(1) - g-cm/s:(1e-05) - g.cm/s:(1e-05) - lb-in/s:(0.0115212) - kg-m/s:(1) - kg.m/s:(1)

Quantity: RotationRate

Reference unit: rad/s
deg/s:(0.0174533) - rpm:(0.10472) - rps:(6.28319) - rad/ns:(1e+09)

Quantity: Moment

Reference unit: N-m
dyn-cm:(1e-07) - lb-in:(0.112985) - lbf-in:(0.112985) - kip-in:(112.985) - nN-nm:(1e-18)

Quantity: Acceleration

Reference unit: m/s2
cm/s2:(0.01) - mm/s2:(0.001) - nm/ns2:(1e+09) - in/s2:(0.0254) - ft/s2:(0.3048)

Quantity: EnergyDensity

Reference unit: J/m3
erg/cm3:(0.1) - lbf/ft2:(47.8867) - lbf/in2:(6895.68) - nJ/nm3:(1) - nnJ/nm3:(1e-09)

Quantity: Power

Reference unit: W
kW:(1000) - MW:(1e+06) - erg/s:(1e-07) - hp:(745.7) - ft-lbf/s:(1.356) - in-lbf/s:(0.113)

Quantity: PowerDensity

Reference unit: W/m3
kW/m3:(1000) - MW/m3:(1e+06) - erg/s-cm3:(0.1) - hp/m3:(745.7) - lbf/s-ft2:(47.8867) - lbf/s-in2:(6895.68)

Quantity: Temperature

Reference unit: degK
degC:(1) - degR:(1.8) - degF:(1.8)

Quantity: TemperatureRate

Reference unit: degK/s
degC/s:(1) - degR/s:(1.8) - degF/s:(1.8)

Quantity: TemperatureInvrs

Reference unit: 1/degK
1/degC:(1) - 1/degR:(0.555556) - 1/degF:(0.555556)

4.2 Actions

These commands are used to schedule various types of tasks to be performed at specific times or steps during the simulation. Each command is entered in a single line of input. These commands are contained in the `ControlParameter` input block.

```
ControlParameters {
  . . .
  FlushTHFiles Every 0.1 ms
  GoInteractive AtTime 10. ms
  WriteRestartFile Every 0.1 ms
  . . .
}
```

4.2.1 Go Interactive

These commands are used to schedule when the program should go interactive. This command is not executed for batch runs.

```
GoInteractive AtTime 10. ms
GoInteractive AtStep 10000
GoInteractive Every 0.1 ms
GoInteractive IfTimeStepLessThan 0.0001 ms
```

4.2.2 Print Progress Line

These commands are used to schedule the printing of a line to the output file. More that one command can be used.

```
PrintProgressLine Frequency 1
PrintProgressLine Frequency 10 Value vmx
// Values can be vmx, ken (default), fmx, wrk
```

4.2.3 Write Restart File

These commands are used to control the frequency for writing restart files. More that one command can be be used.

```
WriteRestartFile AtTime 10. ms
WriteRestartFile AtStep 10000
WriteRestartFile Every 0.1 ms
```

4.2.4 Execute Function

These commands are used to schedule the execution of a macro function. More that one command can be used.

```
ExecFunction 'FunctionName' AtTime 10. ms
ExecFunction 'FunctionName' AtStep 10000
ExecFunction 'FunctionName' Every 0.1 ms
ExecFunction 'FunctionName' IfTimeStepLessThan 0.0001 ms
```

4.2.5 Flush Time Hist Files

These commands are used to schedule when to flush the buffers of the time history datafiles.

```
FlushTHFiles AtTime 10. ms
FlushTHFiles AtStep 10000
FlushTHFiles Every 0.1 ms
```

4.2.6 Read Input File

These command is used to schedule a reading event. At the requestest time or step, MARS will read an input file which contains regular input commands. The input file may be used to add parts to the model, make modifications to the model, write output files, etc.

```
Read 'FileName' atTime 10. ms
Read 'FileName' atStep 10000
```

4.2.7 Write Plot DataFile

These commands are used to schedule when to write database snapshots to the plot data file for later post-processing.

```
WritePlotDatFile data.plt Every 0.1 ms
```

More detail on this procedure are given in the HowTo section.

4.2.8 ExecImplicitSolver

Either command is used for executing the implicit solver at step 0 or at time 0. seconds:

```
ExecImplicitSolver 'solverName' atStep 0
```

```
ExecImplicitSolver 'solverName' atTime 0. s
```

4.3 Time Step Control

The time step used in the MARS explicit time integration scheme can be controlled for both stability and accuracy and is determined by the procedure described in this section. First, MARS computes a Courants time step for each list. This time step is based on the smallest time step for each element in a list. When multiple mechanisms come into play simultaneously, such as contact conditions, penalty constraints, etc, the added stiffness may require for the calculated time step to be further reduced. In general, it is good practice to reduce the time step when a simulation goes unstable. Very often, this is caused by overlapping effects. If this action does not solve the instability, then the instability may be caused by some other reason, such as poor algorithm, possible bug, etc. and the user should notify the developer.

MARS uses the following procedure to determine the time step used in the explicit time integration scheme. First the Courants stability limit `Dtc` is determined list by list and the minimum is selected. The Courants time step is then multiplied by a scaling factor `s` defined via input (default value for `s` is 0.9). The reduced time step is compared to a maximum allowable time step `Dtmax` prescribed via input; the minimum of the two is chosen. chosen.

```
Dt* = s * Dtc
Dt = min (Dt*, Dtmax)
```

The maximum time step `Dtmax` can be defined either as a constant throughout the simulation or as a function of time. The second method is useful when we want the simulation to start with a very small step (for accuracy and not stability like in an impact problem) and then relax this condition as the simulation progresses. progresses.

For constant maximum time step the commands are:

```
ControlParameters {
  Units English
  TimeStepScalingFactor 0.7
  MaximumTimeStep 0.001 ms
  . . .
}
```

For time dependent maximum time step the commands are:

```
ControlParameters {
  Units English
  . . .
}
LoadCurve MaxStepHist {
 // Max allowed time step starts with Dt = 0.1 microsec and grows
  // linearly to 1 microsec in the first ms of the simulation,
  // it remains constant thereafter
  X-Units time ms
  Y-Units time ms
  ReadPairs 3
   0.0   0.0001
   1.0   0.0010
  10.0   0.0010
}
ControlParameters {
  MaximumTimeStepHistory MaxStepHist
}
```

4.4 Plotting Defaults

Plotting defaults are used for initializing the attributes of plottable lists.

```
  PlottingDefaults {
    TimeInterval  0.1 ms [1]
    DisplacementScalingFactor 1000 // [2]
    X-DisplacementScalingFactor 1000 // [2]
    Y-DisplacementScalingFactor 1000 // [2]
    Z-DisplacementScalingFactor 1000 // [2]
    ThickShells
    BinaryPlotFiles
  }
```

[1] This command is used for setting a default time interval for all plot lists. This value can be overwritten inside a `PlotList` input section

[2] These commands are used to magnify displacements. In most large deformation problems, displacement magnification will produce meshes that are too distorted. It can be useful for small deformation problems, like the fracturing of concrete specimens under quasi-static loadings.

4.5 Contact Defaults

Contact defaults are used for initializing some parameters in the contact lists. Currently, only the detection distance parameter and the node/edge/face thicknesses can be specified. The syntax is shown below.

```
ContactDefaults {
  UpdateInterval 0.1 ms // Discontinued (Apr 2011)
  DetectionDistance 0.2 cm
  StaticFriction 0.3  // Discontinued (Apr 2011)
  DynamicFriction 0.2 // Discontinued (Apr 2011)
  NodeThickness 0.1 in
  EdgeThickness 0.2 in
  FaceThickness 0.1 in
}
```

4.6 Global Updates

This command has been added in June 2011. It is meant to replace the updates specified in some lists, such as contact lists, mpi-domain list, etc. The reason for this change is that updates must be synchronized. For example, a contact update and a MPI domain decomposition update must be done at the same time. For this reason, the `UpdateInterval` command in the contact lists will be discontinued.

```
ControlParameters {
  . . .
  GlobalUpdateTimeInterval 0.1 ms
}
```

4.7 Dynamic Relaxation

Dynamic relaxation is a numerical technique that uses an artificial form of damping to dissipate kinetic energy and converge to a steady state equilibrated solution if possible. Dynamic relaxation can be used to compute steady-state stress under static loading conditions in a system before a dynamic load is applied, or find a stable configuration after a dynamic load has been applied. In dynamic relaxation, nodal velocities of all nodes are scaled by a factor slightly less than one. There have been studies that show how to optimize the scaling factor depending on the lowest natural frequency of the system. In

general, if the scaling factor is too small, the simulation overshoots the static solution, possibly resulting in excessive plastic deformations or damage. If the scaling factor is too large (closer to 1.), the convergence rate becomes very slow. There is no magic formula for choosing the optimal scaling factor; the user has to develop a 'feel' for what works best using intuition and a trial-and-error process.In some codes, the scaling factor is specified via input and remains constant throughout the simulation. One disadvantage of this approach is that the damping rate varies with the integration time step. In MARS, the scaling factor is computed as to achieve a desired velocity reduction per unit time (1. microsecond). To make the approach more flexible, the relaxation profile is defined as a function of time in a 'LoadCurve' object. Since the variables of a load curve require dimensional units, the dynamic relaxation command must be specified father down in the input stream, as shown in this example. example.

```
ControlParameters {
  Units English
  . . .
}
. . .
LoadCurve DynRelax {
  X-units time ms
  Y-units nondimensional
  // dyn relax operates in the first ms
  // with velocity reduction of 1% per microsec
  ReadPairs 4
   0.000   0.01
   1.000   0.01
   1.001   0.00
  10.000   0.00
}
ControlParameters {
  ...
  DynamicRelaxationCurve DynRelax // dynamic relaxation
}
```

To stop dynamic relaxation on restart use

```
ControlParameters {
  . . .
  NoDynamicRelaxation
}
```

4.8 Gravity

Gravity loads are automatically computed by specifying a gravity acceleraction. The command can be placed anywhere in the input file after the `ControlParameters` section.

The direction of the acceleration can be prescribed either using one of the three axis labels ('X', 'Y', or 'Z') or more generically using the cosines of a generic direction.

```
ControlParameters {
  . . .
  Gravity -9.8 m/s2 Z
  // or
  Gravity 9.8 m/s2 Direction 0. 0. -1.
}
```

It is possible to apply the gravity load progressively in time using a time history profile. The time history profiles is specified via a load curve, in the same fashion of how it is done for dynamic relaxation. The load curve provides a scaling factor which is multiplied by the value of the acceleration specified after the keyword `Gravity`. In the example below, the gravity is linearly increased from 0 to its final value of 9.8 m/s2 in 2 milliseconds and then it is kept constant.

```
ControlParameters {
  Units English
  . . .
}
. . .
LoadCurve GravityHist {
  X-units time ms
  Y-units nondimensional
  ReadPairs 3
     0.   0.00
     2.   1.00
   100.   1.00
}
ControlParameters {
  ...
  Gravity 9.8 m/s2 Direction 0. 0. -1.  History GravityHist
}
```

4.9 Plugins

By plug-ins, we mean other codes that can be executed from MARS and perform specific tasks. Currently, there are four plug-ins:

- Quasar: for displaying 3-d models
- Xth: for displaying time history plots
- triangle: for generating triangular meshes
- tetgen: for generating tetrahedral meshes

5 Miscellanous Objects

5.1 Reference Systems

Reference systems are used for two main purposes:

1. When generating parts, they are used for aligning a new part in the desired orientation.
2. In finite element formulations, they are used for aligning the local element axis and computing internal strains and stresses.

Three reference systems are available:

1. cartesian,
2. cylindrical, and
3. spherical.

Some applications require the reference system to return a preferential direction, which is used for aligning the first local axis; use the keyword 'return' to select the preferential axis.

5.1.1 Cartesian RefSys

```
ReferenceSystem RSYS cartesian {
  // 1.  Define origin (Opt., default = 0, 0, 0)
  Origin 0.2 in 0.6 in 0. in
  // 2.  Define orientation (Req.)
  FirstDirection 1. 0. 0.
  SecondDirection 0. 1. 0.
  // 3.  Modify  (Opt.)
  Translate 0.4 in 0.3 in 0.6 in
  X-Rotate 45
  // 4.  Select 'Return' direction
  Return X
  // also available Y, and Z
}
```

5.1.2 Cylindrical RefSys

```
ReferenceSystem RSYS cylindrical {
  // 1.  Define origin (Opt., default = 0, 0, 0)
  Origin 0.2 in 0.6 in 0. in
  // 2.  Define orientation (Req.)
  AxialDirection 1. 0. 0.
```

```
  RadialDirection 0. 1. 0.
  // 3.  Modify  (Opt.)
  Translate 0.4 in 0.3 in 0.6 in
  X-Rotate 15 deg
  Y-Rotate 35 deg
  Z-Rotate 180 deg
  // 4.  Select 'Return' direction
  Return HoopDirection // for shells and solids
}
```

5.1.3 Spherical RefSys

```
ReferenceSystem RSYS spherical {
  // 1.  Define origin (Opt., default = 0, 0, 0)
  Origin 0.2 in 0.6 in 0. in
  // 2.  Define orientation (Req.)
  AxialDirection 1. 0. 0.
  RadialDirection 0. 1. 0.
  // 3.  Modify  (Opt.)
  Translate 0.4 in 0.3 in 0.6 in
  X-Rotate 15 deg
  Y-Rotate 35 deg
  Z-Rotate 180 deg
  // 4.  Select 'Return' direction
  Return HoopDirection // for shells and solids
  // also available  AxialDirection, RadialDirection
}
```

5.2 Load Curves

The LoadCurve object is used to prescribe a function of the type $y = f(x)$ in tabulated form by entering (x_i, y_i) pairs. These tabulated functions are used in many algorithms. If during interpolation, the value of x falls outside of the definition range, the value of y is not extrapolated. Instead, it is set to the first or last value in the table. The input data pairs must be in ascending order of x .

```
LoadCurve 'CurveName' {
  // 1. Specify units (Req.)
  X-units time ms
  Y-units pressure psi
  // 2.  Enter tabulated function (Req.)
  ReadPairs 4
  // tim   prss
   0.000     0.
   0.005   100.
```

```
   0.030     0.
   1.000     0.
  // 3.  Modify function (Opt.)
  // the following commands are optional
  X-Scale 2. //  scale x-variable
  X-Offset 0.004 //  offset x-variable
  Y-Scale 2. //  scale y-variable
  Y-Offset 0.004 //  offset y-variable
  Differentiate // differentiate curve [1]
}
```

$z_i = (y_{i+1} - yi - 1)/(x_{i+1} - x_{i-1})$

[1] The `Differentiate` command is used to compute a function which is the differential of the input function

Some common functions can be internally generated in tabulated form. The available functions are listed below: below:

```
LoadCurve 'CurveName' {
  // 1. Specify units (Req.)
  X-units time ms
  Y-units pressure psi
  // 2.  Generate internal function
  // yi = 5. sin(45 xi)  for  xi = i*0.1 and i=0,100
  Generate Sin { A 5. w 45. dt 0.1 n 100 }
  // yi = 5. cos(45 xi)  for  xi = i*0.1 and i=0,100
  Generate Cos { A 5. w 45. dt 0.1 n 100 }
}
```

In time history lists, the current value of a time dependent function can be printed using the command `lc-'curveName` as shown below

```
TimeHistoryList ... {
  . . .
  lc-'curveName'
}
```

5.2.1 Load Curves Lists

It is possible to group a set of load curves that share similar characteristics in a list of load curves (see specific topic in the Misc. section of this manul.) This is the case for reading pressure histories generated by a fluid code.

5.3 Built-In Blast Loads

The built-in blast loads consists of a series of objects that are used in face lists (triangular and quadrilateral faces) for generating pressure loads. Typically, these loads are used for approximating the effects of blast. Pressures are computed taking into account the location of the explosion and the position and orientation of the exposed faces.

5.3.1 ConWep

ConWep is a collection of conventional weapons effects calculations from the equations and curves of TM 5-855-1, 'Design and Analysis of Hardened Structures to Conventional Weapons Effects.' ConWep performs a variety of conventional weapons effects calculations including an assortment of airblast routines, fragment and projectile penetrations, breach, cratering, and ground shock. shock.

The equations used in this special load object are based on a report by Kingery, C.N., and Bulmash, G. 'Airblast Parameters from TNT Spherical Air Burst and Hemispherical Surface Burst', Technical Report ARBRL-TR-02555, U.S. Army ARDC-BRL, Aberdeen Proving Ground, MD, April 1984, and other reports as follows:

1) The following methods are based on the equations from BRL Technical Report ARBRL-TR-02555 for predicting positive phase parameters for either a hemispherical surface burst or spherical free air burst:

```
bool equationsAreNotValid();
real peakIncidentPressure();      // [psi]
real incidentImpulse();           // [psi-ms]
real normallyReflectedPressure(); // [psi]
real normallyReflectedImpulse();  // [psi-ms]
real timeOfArrival();  // time of arrival of blast wave [ms]
real duration();       // time positive phase is done [ms]
real shockFrontVelocity();        // [ft/ms]
real rfp(real p, char tp); // range for given charge and pres. [ft]
real rfi(real i, char ti); // range for given charge and imp. [ft]
real rft(real t, char tt); // range for given charge and time. [ft]
```

2) The following methods, based on the modified Friedlander wave form, are used to determine shape factor, pressure history and dynamic pressure history for the positive phase:

```
real waveShapeFactor(real imp, real pmx, real dt);
real pressureAtTime(real tau, real pmx, real wsf);  // [psi]
real dynPrssAtTime(real tau, real q, real wsf);     // [psi]
```

3) Use the AFWL-70-127 curves to determine the following:

```
real reflectedPressureCoefficient(real alp, real pso);
```

4) Use the TM 5-1300 procedure (Figure 2-192) to find the following:

```
real reflectedImpulseAtAnAngle(real alp);  // [psi-ms]
```

5) Use formula presented by W.E. Baker to determine the following:

```
real peakDynamicPressure(real pso); // [psi]
```

The input commands for specifying this special load are:

```
SpecialLoad BRST ConWep {
  x0 1. in 20. in 0. in
  weight 100 lb
  [ hemispherical ]
  offset 0.012 ms
}
```

The 'offset' parameter is used to offset the time of blast so that the shock wave reaches the exposed surfaces at time zero of the numerical simulation. To compute the optimal offset time, execute the first calculation with an offset of 0. Then, look at the output and it will tell you when the shock wave reaches the surface. Use that value to offset the blast. This operation is done manually because if multiple explosions had to be performed in the same simulation, the user must have the ability to control the relative offset.

5.4 Random Number Distributions

The random number generation object generates random numbers using one of the common distributions equations. Currently, four distributions are available. Random number generators are used for the definition of some inputs. In most cases, the user can select which distribution to use, since they are interchangable.

5.4.1 Weibull distribution

The Weibull distribution has been used very effectivley for characterizing probabilistic failure in materials and mechanical components. The probability density function is defined as

$$P(x) = \frac{g}{a}\left(\frac{x-m}{a}\right)^{(g-1)} \exp\left(-\left(\frac{x-m}{a}\right)^{g}\right) \quad \text{for} \quad x > m, \qquad = 0 \quad \text{otherwise}$$

where where

```
m: location parameter mu
a: scale parameter alpha
g: shape parameter gamma
```

The cumulative distribution function is defined as

$$F(x) = 1 - \exp\left(-\left(\frac{x-m}{a}\right)^{g}\right)$$

The input command is given by

```
Weibull { m 0.4 a 1. g 2 [ n ] }
```

where the optional 'n' is used to normalize the distribution.

5.4.2 Uniform distribution

```
Uniform { d 0.2 }
numbers are generated evenly between 1-d/2 and 1+d/2
```

5.4.3 Gaussian distribution

The Gaussian distribution or normal distribution is a common 'bell shaped' distribution. The probability density function is defined as

```
  PDF(x) = 1/sqrt(2*PI*s^2) exp[-(x-m)^2/2*s^2]
where
  s: standard deviation
  m: mean
```

MARS generates random numbers which are consistent with a Gaussian distribution using the Box-Muller transformation. The Box-Muller Transformation (polar form) generates a pair of random numbers which have a Gaussian distribution with a zero mean and a standard deviation of one. See See
http://www.taygeta.com/random/gaussian.html
The input command is

```
  Gaussian { s 2. m 0.3  mn 0. mx 4. }
where
  mn: is a lower limit
  mx: is un upper limit
```

In other words, random numbers less than 'mn' or larger than 'mx' are rejected. 'mn' and 'mx' are optional inputs.

5.4.4 Fuller distribution

The Fuller/Thompson equation is defined as

```
     P = (d/u)^c
where
     P = percent finer than the sieve
     d = aggregate size being considered
     u = maximum aggregate size to be used
     c = parameter which adjusts curve for fineness or coarseness

Fuller { c 0.5 l 0.4 cm u 1.2 cm [x] }
// c: fuller coefficient
// l: lower value
// u: upper value
// x: examine
```

The distribution is defined in the range of aggregate size between 'l' and 'u', where 'l' is the minimum aggregate size being considered. For maximum particle density, 'c' is approximately 0.5 according to Fuller and Thompson. In the example above, if we consider an aggregate size of 0.8 cm, then $P = (0.8/1.2)^{0.5} = 81\%$ of aggregates are smaller than 0.8 cm. For details, see this web site:

http://training.ce.washington.edu/wsdot/modules/03_materials/03-2_body.htm

5.5 Colors

Colors are used in the definition of surfaces and lines. There are two methods for specifying colors. The first by selecting a color from the built-in list using the command

```
Color Red
```

Available colors are: Red, Green, Blue, Darkgray, Lightgray, Black, Cyan, Steel, Rust, White, Yellow, Orange, Gold, Patina, Clear. The other, by specifying the rgb composition using the command

```
Color rgb 0.4 0.6 0.2
```

where the three numbers following the 'rgb' keyword indicate the brightness of each color (red, green, blue in this order) on a scale from 0 to 1.

5.6 Strain Gages

The `StrainGage` object is designed to simulate the behavior of actual strain gages. As such, it can provide a more realistic measurement of local deformations for comparison with test data than the various strain metrics from continuum mechanics. The strain gage object is defined by selecting two or more material points inside or on the surface of a part. The points are placed in correspondence of where the physical strain gage is placed. While physical strain gage are only placed on the surface of a part, these numerical strain gage can be also placed in the interior of a part. The numerical strain gage is defined using its location, length, and direction.

The main purpose of the numerical strain gage is to produce a time history record of the local strain which can be used for comparison with test data or just for better understanding of the results from the simulation. The numerical strain gage computes the a total length by summing the lengths of the segment[s] used in the definition. The length L0 at time 0 is assumed to be the reference length at rest of the strain gage. The linear strain eps(t) at time t is defined as eps(t) = (L(t)/L0) - 1, where L(t) is the strain gage length at time t. The logarithmic strain is defined as eps(t) = ln(L(t)/L0).

The structure of a typical strain gage input is shown below.

```
StrainGage 'GageName' {
  // part on which the strain gage is attached to
  // type dependent parameters
  . . .
}
```

More details on how to place strain gages on various types of meshes are discussed in the subsections below.

5.6.1 Strain-Gage for hexahedral solid lists

Currently, strain gages can only be placed on the surface of a hex solid element mesh. Typical input is shown below:

```
StrainGage GageX {
  hxL 'HexPartName'  // or HexSolidList 'HexPartName'
  Description Strain gage at location X5
  CenterAt 0. cm 10. cm 9. cm
  Length 2. cm
  Segments 3
  Direction 0. 1. 0.
}
```

5.6.2 Strain-Gage for tetrahedral solid lists

Strain gages can only be placed on the surface or in the interior of a tet solid element mesh. Typical input is shown below:

```
StrainGage GageX {
  TetSolidList Solid
  Description Strain gage at location X5
  CenterAt 0. cm 0. cm 0. cm
  Length 2. cm
  Segments 3
  Direction 0. 1. 0.
}
```

5.6.3 Strain-Gage for quadrilateral shell lists

Strain gages can be placed on the top surface, bottom surface, or mid-plane (membrane strains) of a quadirlateral shell element mesh. Typical input is shown below:

```
StrainGage SGx {
  qsL 'ShellPartName'  // or QuadShellList 'ShellPartName'
  Description Strain gage at location X5
  CenterAt 0. cm 10. cm 9. cm
  TopSurface  // also 'BottomSurface'  [1]
  Length 2. cm
  Segments 3
  Direction 0. 1. 0.
}
```

[1] If neither `TopSurface` or `BottomSurface` keyword is specified, then the default is mid-plane surface for computing membrane strains.

5.6.4 TimeHistories

The strain gage computes a single variable: the total strain at the prescriped point over a prescribed length. The only purpose of a `StrainGage` is to provide a measurement of local strain for time history lists. Typical application show up as

```
StrainGage Gage1 {
  . . .
}
 . . .
TimeHistoryList HIST {
  . . .
  sg-Gage1 linear S 1000. //  'linear' or 'logarithm' [1]
}
```

[1] The keywords `linear` and `logarithm` are used to specify how strains are computed and it makes a difference mostly for large deformations. Default is `linear`.

5.7 Accelerometer

The `Accelerometer` object is designed to simulate the behavior of actual accelerometers for direct comparisons with acceleration records measured in test setups. The acceleration computed by the Accelerometer object employs a corotational formulation suitable for large rotations. As such, it may be different than the acceleration computed at the nodes in the global fixed reference system. While physical accelerometers are only placed on the surface of a part, these numerical accelerometers can be also placed in the interior of a part. The numerical acceleration is defined using its location, length, and direction.

The main purpose of the numerical accelerometer is to produce a time history record of the local acceleration which can be used for comparison with test data or just for better understanding of the results from the simulation. Accelerations are computed as follow

$$a_n = \frac{\vec{v}(t) - \vec{v}(t - \Delta t)}{\Delta t} \cdot \vec{n}$$

where n is the corotational direction aligned with the accelerometer.

There are two types of numerical accelerometer: 1. Those attached to a finite element component, 2. Those embedded in a discrete element model (cloud of points).

Typical input is shown below.

```
Accelerometer 'GageName' type {
  // part on which the strain gage is attached to
  // type dependent parameters
  . . .
}
```

More detailed input on how to place an accelerometer on various types of meshes are discussed in the subsections below.

5.7.1 Attached to quadrilateral surfaces

```
Accelerometer AG01 QuadFace {
  FaceList OuterPlate
  Description Accelerometer AG-01
  CenterAt 0. in 10. in 9. in
  Tolerance  0.01 in
  Direction 0. 0. 1
}
```

5.7.2 Attached to triangular surfaces

```
Accelerometer AG01 TriangFace {
  FaceList OuterPlate
  Description Accelerometer AG-01
  CenterAt 0. in 10. in 9. in
  Tolerance  0.01 in
  Direction 0. 0. 1
}
```

5.7.3 Attached to the surfaces of a beam element

```
Accelerometer AG01 Beam {
  BeamList OuterPlate
  Description Accelerometer AG-01
  CenterAt 0. in 10. in 9. in
  Tolerance  0.01 in
  Direction 0. 0. 1
}
```

5.7.4 TimeHistories

The accelerometer computes a single variable: the acceleration component at the prescriped point in the prescribed corotational direction. The only purpose of an `Accelerometer` is to provide acceleration for time history lists. Typical application show up as

```
Accelerometer Gage1 QuadFace {
  . . .
}
 . . .
TimeHistoryList HIST {
  . . .
  ac-Gage1
}
```

5.8 Equations

This is a collection of objects that implement global equations, such as pressure-volume equations, etc.

5.8.1 Pressurized Volume

```
Equation 'name' PressurizedVolume {
  InitialVolume  34.53 cm3
  InjectionHistory 'name2'
  // Enter the name of fluid or BulkModulus
  Oil / Water / Air
  Temperature 70 degF
}
```

5.8.2 Injected Fluid

Use this equation when ... Work still in progress

```
LoadCurve 'name2' {
  // Specify flow rate history
  . . .
}
Equation 'name' InjectedFluid {
  InitialVolume  34.53 cm3
  InjectionHistory 'name2'
  // Enter the name of fluid or BulkModulus
  Oil (K = 1.5e9 Pa) / Water (K = 2.2e9 Pa) / Air (1.42e5 Pa)
  BulkModulus 10e6 psi
}
```

5.8.3 Adiabatic Compression

This feature was inserted in the code in the spring of 2009. The purpose of this feature is to enable the numerical simulation of the effect of air trapped inside a cavity whose volume changes during the simulation. The pressure in the cavity is related to the change in volume using the adiabatic equation:

$$p(t)V(t)^{\gamma} = \text{const}$$

where $p(t)$ is the pressure, $V(t)$ is the volume of the cavity, and γ is the adiabatic index of the gas. The ability to model these conditions was introduced into the MARS code through a new C++ class denoted as `AdiabaticEquation` . This class is derived from the base class `Equation` . The 'AdiabaticEquation' class implements the very simple adiabatic equation:

$$p(t) = (V_0/V(t))^{\gamma} p_0$$

where p_0 and V_0 are the initial value of the pressure and volume respectively. The method implemented in Mars actually returns the overpressure, which is defined as

$$p_o(t) = p(t) - p_0$$

The input block requires three parameters as shown below:

```
Equation 'name' AdiabaticCompression {
  InitialVolume  34.53 cm3
  InitialPressure  14.7 psi
  Gamma 1.4
  [ InvertSign ]
}
```

The `InvertSign` command should be used when the surfaces point toward the cavity rather than away from it.

5.9 Material Models

5.9.1 Elastic Material Model

The elastic material model implements the simplest forms of constitutive equations in three main formats: tensorial, plane stress (for shells), and vectorials (for beams).

```
Material ELST elastic {
  Description  Stainless Steel ...
  Density 7.8 g/cm3
  YoungsModulus 29e6 psi
  PoissonsRatio 0.3
}
```

State variables for tensorial equations

```
 1: XX-Stress [stress]
 2: YY-Stress [stress]
 3: ZZ-Stress [stress]
 4: YZ-Stress [stress]
 5: ZX-Stress [stress]
 6: XY-Stress [stress]
```

State variables for plane stress equations

```
 1: XX-Stress [stress]
 2: YY-Stress [stress]
 3: YZ-Stress [stress]
 4: ZX-Stress [stress]
 5: XY-Stress [stress]
```

State variables for vectorial equations

```
 1: "Normal stress" [stress]
 2: "Shear stress X" [stress]
 3: "Shear stress Y" [stress]
```

5.9.2 Elastio-plastic Material Model

```
Material PLST plastic {
  Description  Stainless Steel ...
  Density 7.8 g/cm3
  YoungsModulus 29e6 psi
  PoissonsRatio 0.3
  YieldStress 80e3 psi
  HardeningModulus 200e3 psi
#-- select one of the three hardening options below
  IsotropicHardening
  KinematicHardening
  Beta 0.5 //  beta = 0 istropic, beta = 1 kinematic
  hmx 8e3 psi // Bounding stress for friction damping
}
```

'Friction' damping provides hysteretical energy loss for each cycle related to cycle amplitude and not strain rate. Because it is non-viscous the term 'friction' damping is used. Use a bounding stress in the order of one percent of the yield stress if damping is desired.

State variables for tensorial equations

```
 1: XX-Stress [stress]
 2: YY-Stress [stress]
 3: ZZ-Stress [stress]
 4: YZ-Stress [stress]
 5: ZX-Stress [stress]
 6: XY-Stress [stress]
 7: Effective plastic strain [nondimensional]
 8: XX-Back stress [stress]
 9: YY-Back stress [stress]
10: YZ-Back stress [stress]
11: ZX-Back stress [stress]
12: XY-Back stress [stress]
13: XX-Friction stress [stress]
14: YY-Friction stress [stress]
15: ZZ-Friction stress [stress]
16: YZ-Friction stress [stress]
17: ZX-Friction stress [stress]
18: XY-Friction stress [stress]
```

```
19: XX-Strain [nondimensional]
20: YY-Strain [nondimensional]
21: ZZ-Strain [nondimensional]
22: YZ-Strain [nondimensional]
23: ZX-Strain [nondimensional]
24: XY-Strain [nondimensional]
25: Energy [energy]
```

State variables for plane stress equations

```
 1: XX-Stress [stress]
 2: YY-Stress [stress]
 3: YZ-Stress [stress]
 4: ZX-Stress [stress]
 5: XY-Stress [stress]
 6: Effective plastic strain [nondimensional]
 7: XX-Back Stress [stress]
 8: YY-Back Stress [stress]
 9: YZ-Back Stress [stress]
10: ZX-Back Stress [stress]
11: XY-Back Stress [stress]
12: XX-Friction Stress [stress]
13: YY-Friction Stress [stress]
14: YZ-Friction Stress [stress]
15: ZX-Friction Stress [stress]
16: XY-Friction Stress [stress]
```

State variables for vectorial equations

```
 1: "Normal stress" [stress]
 2: "Shear stress X" [stress]
 3: "Shear stress Y" [stress]
 4: "Effective plastic strain" [nondimensional]
```

5.9.3 Rate Sensistive Elasto-plastic Material Model

```
Material PLST plastic {
  Description  Stainless Steel ...
  Density 7.8 g/cm3
  YoungsModulus 29e6 psi
  PoissonsRatio 0.3
  YieldStress 80e3 psi
  HardeningModulus 200e3 psi
#-- select one of the three hardening options below
  IsotropicHardening
  KinematicHardening
```

```
  Beta 0.5 //  beta = 0 istropic, beta = 1 kinematic
  D1 100. // [1/s]  strain rate for intermediate point
  sy1 90e3 psi   // yield stress for intermediate point
  syi 100e3 psi  // yield stress for infinite strain rate
}
```

5.9.4 Johnson-Cook Model

The Johnson-Cook model is purely empirical and gives the following relation for the flow stress

$$\sigma_y(\epsilon_p, \dot{\epsilon}_p, T) = (A + B(\epsilon_p)^n)\left(1 + C\ln\left(\dot{\epsilon}_p^*\right)\right)(1 - (T^*)^m)$$

where

σ_y is the flow stress
ϵ_p is the equivalent plastic strain
A, B, C, n, and m are material constants
ϵ_p^* is the normalized strain-rate
T^* is the normalized temperature

The normalized strain-rate and temperatures in the equation above are defined as

$$\dot{\epsilon}_p^* = \frac{\dot{\epsilon}_p}{\dot{\epsilon}_{p0}} \qquad \text{and} \qquad T^* = \frac{T - T_0}{T_m - T_0}$$

The input commands for specifying the material parameters are

```
Material PLST JohnsonCook {
  Description  Stainless Steel ...
  Density 7.8 g/cm3
  YoungsModulus 29e6 psi
  PoissonsRatio 0.3
  A 80e3 psi
  B 80e3 psi
  C 4.
  n 4.
  m 4.
  ReferencePlasticStrainRate 0.0001 1/s
  ReferenceTemperature 40 degC
}
```

This material model is available fos solids, shells, beams, and trusses. The following materials have built-in properties which were found in the literature

```
Material PLST JohnsonCook {
  Steel-1045
```

```
  Steel-4340
  Al6082-T6
  Ti6Al4V
}
```

To plot stress strain curves for different strain rates use the `Test` command, e.g.

```
Material PLST JohnsonCook {
  Steel-1045
  Test Tensor Tension
}
```

which generates a time history file named `mat.th`.

5.9.5 LDPM Concrete Material Model

```
Material CONC RCConcrete Dev {
  MixDesign {
    Density 2.400 g/cm3
    CementContent 300 kg/m3
    WaterToCementRatio 0.5
    AggregateToCementRatio 6.0
    MinAggregate 10.0 mm
    MaxAggregate 16.0 mm
    FullerCoefficient 0.5
  }
  StaticParameters {
    NormalModulus 50000 MPa  // nmo
    DensifcationRatio 1.0  // nmo
    Alpha 0.25
    TensileStrength 3.0 MPa  // ftm
    CompressiveStrength 50 MPa  // fcm
    ShearStrengthRatio 2.5  // fsm
    TensileCharacteristicLength 100 mm // tcl
    SofteningExponent 0.25 //ncm
    InitialHardeningModulusRatio 0.33 MPa // IHm
    TransitionalStrainRatio 5.0 // hts
    InitialFriction 0.4 // mu0
    AsymptoticFriction 0.0 // mui
    TransitionalStress 50.0 MPa // fts
    VolumetricDevitoricCoupling 0.0 // beta
    DeviatoricStrainThresholdRatio 0.5 // dk1
    DeviatoricDamageParameter 5.0 // dk2
  }
  StrainRateEffect {
    PseudoTimeFactor 1.0 //  {1}
```

```
    ReferenceStrainRate 1E-6 1/s  // cc0
    RateEffectParameter 5E-2  // cc1
  }
}
```

1 The PseudoTimeFactor is used to correctly integrate the constitutive equation while using a fictitiously higher rate of loading for the simulation. For example, assume that you have an experimental test in compression on a specimen loaded at 0.01 in/sec. In this case you have rate effect on the constitutive equation (and the macroscopic behavior) but the inertia effects are likely to be small or negligible (compared to the internal energy, a ratio of about 1000 is typically fine). Then you may decide to run the simulation at (for example) 0.2 in/sec to save computational time while not changing significantly the kinetic energy (compared to the internal energy). However if you do so you need to make sure that the constitutive equation 'feels' a loading rate of 0.01 in/sec otherwise you would not get the response associated with 0.01 in/sec which is what you want. You make the constitutive law 'feeling' 0.01 in/sec even if you run at 0.2 in/sec by setting the PseudoTimeFactor = 0.2 / 0.01 = 20. 20.

State variables for vectorial equations

```
 1: "Normal N stress" [stress]
 2: "Shear M stress" [stress]
 3: "Shear L stress" [stress]
 4: "Normal N strain" [nondimensional]
 5: "Shear M strain" [nondimensional]
 6: "Shear L strain" [nondimensional]
 7: "Max normal N strain" [nondimensional]
 8: "Max shear T strain" [nondimensional]
 9: "Tensile strength" [stress]
10: "Post-peak slope in tension" [stress]
11: "Shear L crack opening" [length]
12: "Volumetric Strain" [nondimensional]
13: "Normal N crack opening" [length]
14: "Shear M crack opening" [length]
15: "Total crack opening" [length]
16: "Facet failure flag" [nondimensional]
17: "Dissipated energy density rate" [powerDensity]
18: "Dissipated energy density" [energyDensity]
19: "Dissipated energy density rate in tension" [powerDensity]
20: "Dissipated energy density in tension" [energyDensity]
```

5.9.6 RCI Rebar-Concrete Interaction Model

```
Material  RCI RebarConcreteInteraction {
  StaticParameters {
    ...
```

```
  }
  StrainRateEffects {
    ...
  }
}
```

State variables for vectorial equations

```
 1: "Axial stress" [stress]
 2: "Radial stress" [stress]
 3: "Circumf. stress" [stress]
 4: "Axial slippage" [length]
 5: "Radial slippage" [length]
 6: "Circumf. slippage" [length]
 7: "Max. axial slippage" [length]
```

5.9.7 LDPM Concrete-Fiber Interaction Model

This model is used exclusively for computing concrete-fiber interaction at the LDPM cell factes. It should not be used with any of the finite element formulations.

```
Material CFI LdpmFiber Dev {
  ElasticModulus              210000 MPa   // ymf,
  SpallingParameter             1500 MPa   // sps,
  FiberStrength                 1172 MPa   // sfu,
  FiberStrengthDecay               0.0     // fsd,
  SnubbingParameter                0.05    // fsn,
  BondStrength                     1.75 MPa // tau,
  VolumeStiffnessRatio             0.0     // eta
  DebondingFractureEnergy          0.1 N/m // gdm,
  PullOutHardening                 0.05    // poa
  CookGordonParameter              2.
  SpallingParameter               150  MPa
}
```

State variables for vectorial equations

```
 1: "Normal N force" [force]
 2: "Shear M force" [force]
 3: "Shear L force" [force]
 4: "Normal N strain" [nondimensional]
 5: "Shear M strain" [nondimensional]
 6: "Shear L strain" [nondimensional]
 7: "Short side slippage" [length]
 8: "Long side slippage" [length]
 9: "Max short side slippage" [length]
```

```
10: "Max long side slippage" [length]
11: "Spalling length" [length]
12: "Cook-Gordon crack opening" [length]
13: "Failure flag" [nondimensional]
14: "Dissipated energy" [energy]
15: "Normal crack opening" [length]
16: "Shear M crack opening" [length]
17: "Shear L crack opening" [length]
```

5.9.8 Simple Cap Concrete Material Model

```
Material PLST SimpleCap {
  Description  Simple concrete model
  Density 2.0 g/cm3
  YoungsModulus  4e6 psi
  PoissonsRatio 0.3
  BulkModulus 0.3
  ShearModulus 0.3
  // Fe = alpha + theta*I  failure curve
  Alpha 0.07
  Theata 0.07
  X0 3000 psi  // initial cap location
  W 0.07       // void ratio
  // select one of the blocks below
  // 1) epv = W epx( - D1 (X-X0) )
  D1  0.001    // make sure it is givne in 1/stress
  // 2) epv = W epx( - D2 (X-X0)^2 )
  D2  0.001    // make sure it is given in 1/(stress)2
  // 3) epv = W (I-X0) / (X1-X0)
  X1 40e3 psi  // lock-up
}
```

5.9.9 K&C Concrete Material Model

The K&C material model was inserted in Mars in 2003 and it has not been updated since. In its simplest input form, only three parameters are necessary to specify material properties.

```
Material Concrete KcConcreteModel {
  Density 2.0 g/cm3
  PoissonsRatio 0.19
  CompressiveStrength 6000 psi
}
```

All other parameters and curves are automatically generated. If the user wants to refine material parameters to match specific data, the following addtional parameters can be specified.

```
LoadCurve Curve1 {
  // volumetric strain versus bulk modulus curve
  . . .
}
LoadCurve Curve2 {
  // pressure versus volumetric strain curve  . . .
}
LoadCurve Curve3 {
  // strain-rate enhancement curve
  . . .
}
Material Concrete KcConcreteModel {
  Density 2.0 g/cm3
  PoissonsRatio 0.19
  CompressiveStrength 6000 psi
  TensileStrength 600 psi
  BulkModCurve Curve1
  PressureCurve Curve2
  StrainRateEnhancement Curve3
  OneInch 1. // [2]
}
```

The user can enter partial data, for example `Curve1` but not `Curve2` and `Curve3`. The program will automatically generate data only for the missing data
[2] The parameter `OneInch` was used for telling the model the units used in the calculations. For example, if the calculation employs cm as length units, the value of `OneInch` would be 2.54. This parameters should be no longer needed since all input values are now entered with their dimensions.

5.10 Functions / Macros

The Functions object makes it possible to write a script and perform operation on the objects of the database. Variables in the database are accessed using the same convention that is used to identify variable for time history plotting.

```
Function  FNC1 {
  . . .
}
exec FNC1 now
```

The Function can be also invoke by the `Action` scheduler.

```
Function  'FunctionName' {
  . . .
}
ControlParameters {
```

```
  . . .
  ExecFunction 'FunctionName' AtTime 10. ms
  ExecFunction 'FunctionName' AtStep 10000
  ExecFunction 'FunctionName' Every 0.1 ms
  ExecFunction 'FunctionName' IfTimeStepLessThan 0.0001 ms
```

Following are some examples of scripts that can be performed in a function. The first script converts a flat plate into a cylindrical shell.

```
Function  FNC1 {
  silent // do not display message when executing function
  int nnd
  real cx
  real cy
  real cz
  real dangle
  dangle = 3.14159 / 24.
  real angle
  real cs
  real sn
  nnd = ndL-PLAT num
  int i
  do i = 1 $nnd [
    cz = nd-PLAT $i cx
    cy = nd-PLAT $i cy
    angle = $cz * $dangle
    print angle   // debug printing
    cs = cos angle
    sn = sin angle
    cx = $cs * $cy
    cy = $sn * $cy
    cx = -1. * $cx
    cy = -1. * $cy
    print cx
    print cy
    nd-PLAT $i cx = $cx
    nd-PLAT $i cy = $cy
    nd-PLAT $i cz = $cz
  ]
}
exec FNC1 now
```

The second example moves nodes that are outside of a cylinder of radius `R0` to the surface of the cylinder.

```
Function TRIM {
```

```
  int nnd
  real cx
  real cy
  real tm
  real rd
  real R0
  nnd = ndL-TPOL num
  R0 = 27.75 / 2.
  print nnd
  int i
  logical lg
  do i = 1 $nnd [
    cx = nd-TPOL $i cx
    cy = nd-TPOL $i cy
    tm = $cx * $cx
    rd = $cy * $cy
    rd = $rd + $tm
    rd = sqrt rd
    lg = $rd > $R0
    if ( lg ) [
      print rd
      print R0
      tm = $R0 / $rd
      cx = $cx * $tm
      cy = $cy * $tm
      nd-TPOL $i cx = $cx
      nd-TPOL $i cy = $cy
    ]
  ]
}
exec TRIM now
//  functions (observe spaces)
  real x
  real y
  y = random // random number between 0 and 1
  y = sin ( $x )
  y = cos ( $x )
  y = abs ( $x )
  y = sqrt ( $x )
```

The third example checks the maximum Von Mises stress in a list of hexahedral elements every microsecond. When the max Von Mises stress exceed and ultimate material stress `Ftu`, the calculation stops and the code is instructed to print various information.

```
Function F1 {
```

```
  silent
  real Ftu
  real syP
  real Mx
  logical lg
  Ftu = 67000.
  syP = hxL-Pin MaxVonMisesStress
  lg = $syP > $Ftu
  if ( lg ) [
    Mx = RB-X2 mx
    echo -------------------------------------------
    echo Final results
    print su
    print Ftu
    echo Mx: moment at failure
    print Mx
    echo -------------------------------------------
    QUIT
  ]
}
ControlParameters {
  ExecFunction F1 every 0.001 ms
}
```

The output at the end of the run looks like this

```
-------------------------------------------
Final results
Ftu = 67000
Mx: moment at failure
Mx = -1.78388e+06
-------------------------------------------
```

5.11 Pre-Set Test Simulations

This is a collection of objects for performing simulations of simple tests, such as concrete biaxial, triaxial, or Colorado tests.

5.11.1 Biaxial Test

```
//  Model restrictions:
//   1) Specimen must be a cube or a prism
//   2) Displacements imposed on plates perpend. to z-axis
//   3) Ratioed forces imposed on plates perpend. to x-axis
Test 'TestName' Biaxial {
```

```
  TetSolidList 'Specimen'  // specimen list
  VelocityHistory 'History'
  StressRatio  0.5 //  lateral over vertical
}
TimeHistoryList HIST {
  teL-'TestName' VerticalStress
  teL-'TestName' VerticalStrain
  teL-'TestName' HorizontalStress
  teL-'TestName' HorizontalStrain
}
```

5.11.2 Triaxial Test

```
//  Model restrictions:
//   1) Specimen must be a cube or a prism
//   2) Displacements imposed on plates perpend. to z-axis
//   3) Ratioes forces imposed on plates perpend. to x- and y-axis
Test 'TestName' Triaxial {
  TetSolidList 'Specimen'  // specimen list
  VelocityHistory 'History'
  XStressRatio  0.5 //  lateral over vertical
  YStressRatio  0.5 //  lateral over vertical
}
TimeHistoryList HIST {
  teL-'TestName' VerticalStress
  teL-'TestName' VerticalStrain
  teL-'TestName' XHorizontalStress
  teL-'TestName' XHorizontalStrain
  teL-'TestName' YHorizontalStress
  teL-'TestName' YHorizontalStrain
}
```

5.11.3 Colorado Test

```
ReferenceSystem RSYS cartesian {
//  Model restrictions:
//   1) The geometry is a 4-inch side cube
//   2) The center of the cube is at the origin
Test BXCT Colorado {
  TetSolidList CUBE
  X-PressureHistory PTHX
  Y-PressureHistory PTHY
  Z-PressureHistory PTHZ
}
```

6 Nodes and Particle Lists

6.1 Node Lists

In MARS, nodes and spherical particles are used interchangably. The same class (in the OOL sense) is used for both entitites. A typical input block for specifying a node-list is shown below:

```
NodeList 'ListName' {
  Read filename // read nodelist command from file
  // if this list is used to define a rigid body, enter
  Density 7.8 g/cm3
  // if this is a DP tet list, enter
  Particles
  Color Red
  LengthUnits cm
  VelocityUnits cm/s  // if velocities are entered
  InputFormat IXYZR   // index, cx, cy, cz, and rd
  // available input formats below (B boundary code, UVW velocities)
  //    IXYZ IBXYZB IXYZR XYZ IXYZRUVW
  // Boundary condition code:  XOO = fix cx, free cy and cz
  ReadNodes 345
  // if InputFormat = IXYZR then
  //  i   cx   cy   cz   rd
      1  1.4  2.4 -4.5 0.12
      2  1.8  2.1 -4.2 0.17
      . . .
  // else if InputFormat = IBXYZB then
  //  i  trn    cx   cy   cz  rot
      1  OOX   1.4  2.4 -4.5  OOO
      2  XXX   1.8  2.1 -4.2  OOO
      . . .
  Select ...  // select nodes from list, see below
  Set ...  // set values on selected nodes, see below
  Scale 0.4    // scale all cords by 0.4
  X-Scale 0.4  // scale in x-direction only
  Y-Translate 0.4 in
  Z-Rotate 45 // rotate sel nodes 45 deg about z-axis
  Move 0.3 in 0.5 in 0.3 in
  StructuralDamping 0.001 1/s // to be implemented
  PlotAttributes { ... } // see below
  ComputePackingRatio 'lengthUnits' 'xmn' 'xmx' 'ymn' 'ymx' 'zmn' 'zmx'
  // extract a node subset
  Extract Dogbone { . . . }
  Make NodeList SubListName
```

```
  Write NodeDataFile PartNodes.mrs
  CoordinateOutputFormat %10.6f
}
```

6.1.1 Select Commands

Select commands make it possible to select a subset of nodes using various criteria. The selection can be immediately used for imposing conditions or saved with a name for later processing.

```
  Select [criteron]
  AlsoSelect [criteron]
  Unselect [criteron]
  Reselect [criteron]
  InvertSelection // invert current node selection
  SaveSelection 'selection name'
  // [criterion] can take the following forms
  // all    // all nodes
  // do 25  // node 25
  // do 1 5 // node 1 through 5
  // do 1 100 2 // nodw 1 through 100 step 2
  // cx < 0.4 in // nodes with cx < 0.4
  // cy = 0.4 cm // nodes with cy apprx = 0.4
  // tb = OOX    // nodes with translational BC = OOX
  // rb = XXX    // nodes with rotational BC = XXX
  // vz > 10 m/s // nodes with z-velocity > 10
  // cl  0. 10. 4. cm // node closest to point (0.,10.,4.)
// Examples:
  Select do 1 100 // select nodes 1 through 100
  AlsoSelect do 201 300 // add nodes 201 - 300
  Reselect cx < 0. in // select nodes with negative x
                      // from nodes already selected
```

Nodes can also be selected from within element lists. Following are a few examples. The first example shows how to select nodes that belong to a set of faces which point in the positive x-direction. These could be all the nodes of a circular face of a cylinder aligned with the x-axis.

```
TriangFaceList 'ListName' {
  . . .
  EditNodeList {
    Unselect all
  }
  Select  FacesWithCrossProduct 1. 0. 0. > 0.99
  SelectNodes
  EditNodeList {
```

```
    Set Translations XXX
    Select all
  }
}
```

Most element lists provide the following commands: 'SelectNodes', 'UnselectNodes', and 'ReselectNodes'. The second example shows the difference between 'SelectNodes' and 'ReselectNodes'; in the example, we want to select nodes that are shared by two element lists and save them in a new node list (Refer to 'other commands').

```
NodeList Nodes {
  Unselect all
}
TriangShellList Shells {
  SelectNodes
}
HexSolidList Solids {
  ReselectNodes
}
NodeList Nodes {
  Make NodeList CommonNodes
}
```

For the nodes to be selected, they have to be used in both element lists (intersection of the two sets). If we had used 'SelectNodes', in the HexSolidList, then the selected nodes would include all nodes from both lists (union of the two sets).

6.1.2 Set Commands

The 'Set' command is used to set variables or boundary conditions on a set of nodes that was previously selected using the 'Select' commands. If no selection was previously done, then the 'Set' command will operate on all nodes.

```
NodeList 'ListName' {
  . . .
  Set TranslationsBC XXX
  Set RotationsBC XXX
  Set X-Velocity 100 in/s
  Set Y-Rotation 100 1/s
  Set Radius 0.3 in
}
```

6.1.3 Scale Commands

Scale commands make it possible change node coordinates and particle radii by multiplying them by a constant factor. For example, the command

```
Scale 1.4
```

multiplies x-, y-, z-coordinates and radii of all selected nodes by the value 1.4. If different scaling factors are desired in different directions, these commands may be used:

```
X-Scale 1.2
Y-Scale 1.4
Z-Scale 1.1
R-Scale 0.9 // scale particle radii by 0.9
```

6.1.4 Translate/Rotate Commands

Translate/Rotate commands are used to move and reorient a set of nodes. These commands are executed during the reading phase, in the order in which they appear. This is important, because a rotation after a translation gives different results than the same translation after the same rotation

```
X-Translate 3 cm
Z-Rotate 90 deg
```

A mesh can be simultaneoulsy translated in all three direction using the 'Move' command:

```
Move 3 cm 0. cm 5 cm
```

A special case of the translate command is the 'Align' command:

```
X-Align Min   //  { Min / Max / Center }
```

In this case, the code computes the mininum x-coordinate and shifts the mesh in the x direction so that the minimum coordinate becomes 0. Also available are 'Y-Align' and 'Z-Align'. If 'Max' is used instead of 'Min', then the mesh is aligned so that the maximum x-coordinate is 0. If 'Center' is used, the mesh is centered around the 0. x-value.

6.1.5 Other Commands

The 'Make NodeList' command is designed to create a new node list that contains references to the nodes selected in the current list. The new list is 'passive', in other words, the list does not 'own' the nodes and does not perform any active operation on them, such as integrating the equation of motion. However, the node selection can be used for many purposes:

1. the nodes can be used in time histories.
2. the nodes can be used to set boundary conditions.

6.1.6 Time History Commands

The following line commands are intended to be used inside Time History lists to produce records of global and element variables.

```
TimeHistoryList HIST {
  . . .
  ndL-NODS ke
  nd-NODS 155  vx
  nd-NODS cl 0.1 in 0.5 in 0.4 in  vx
  // list labels for available quantities
  // (in parenthesis, value for entire list: CG = values at CG,
        I = volume integral)
  // cx: x coordinate (CG)
  // cy: y coordinate (CG)
  // cz: z coordinate (CG)
  // vx: x velocity (CG)
  // vy: y velocity (CG)
  // vz: z velocity (CG)
  // fx: x force (I)
  // fy: y force (I)
  // fz: z force (I)
  // mx: x moment (I)
  // my: x moment (I)
  // mz: x moment (I)
  // wx: x rotation rate (CG)
  // wy: x rotation rate (CG)
  // wz: x rotation rate (CG)
  // vl: absolute velocity (CG)
  // ke: kinetic energy (I)
  // px: x momentum (I)
  // py: y momentum (I)
  // pz: z momentum (I)
  // ax: x angular momentum (I)
  // ay: y angular momentum (I)
  // az: z angular momentum (I)
```

6.1.7 Plot List Commands

It is possible to generate plot files for Quasar and Paraview of various node variables. The input commands for the two post-processors are quite different. The main difference is that for Quasar files you have to preselect the information you want to plot but it can be combined with other lists. For Paraview, most of the nodal information is written to the file and the appearance for the plot is chosen during post-processing. Although it is still possible to set plot attributes for Quasar plots within a `NodeList` section, this is no longer recommended. Quasar plot attributes should be entered in the `PlotList` section.

```
PlotList PLOT {
  TimeInternval 0.1 ms
  ndL 'NodeListName' {
    // 1.  Select resolution [optional, default = Low]
    HighResolution
    MediumResolution
    LowResolution
    // 2.  Set or change node/particle radii [optional]
    scl 0.5  // scale particle size by 0.5
    MinRadius 0.5 in
    // 3.  Select contour variable [optional]
    var  vx  // plot fringe plots of x-velocity
    vmn   0. // bottom value for fringe plots [1]
    vmx 100. // top value for fringe plots [1]
    // 4.  Change displacement scale [optional]
    DisplacementScalingFactor 1000. // <dsf 1000.>
}
```

[1] The minimum and maximum values for the range are not required. For each plot, MARS computes the minimum and maximum of the quantity to be plotted. Either one or both are overwritten if the min and/or max are specified in the input. By fixing the range, it is possible to make animation movies where the colors are consistent across frames.

Plotting command for Paraview files are simpler. First, recall that it is preferable to have one list per plot file. Second, all other parameters except `DisplacementScalingFactor` are controlled within Paraview

```
PlotList 'PlotListName' {
  Paraview
  TimeInterval 0.1 ms
  ndL 'NodeListName' { }
}
```

Velocity and rotation vectors of selected nodes/particles are automatically saved in Paraview files. The Paraview procedure for displaying particles and velocity (or rotation rate) vectors as arrows is described below:

```
Main Menu: [File]->[Open]  Select files Particles.00*
Pipeline Browser: Click on Particles.00*
Object Inspector: (Properties) (Apply)
--  Display particles as gray spheres
Main Menu: [Filters]->[Recent]->[Gliph]
Object Inspector:
  In Properties:
    Glyph Type: Sphere
```

```
    Scale Mode: scalar
    Set Scale Factor: check Edit box and enter 0.5
    Radius: 1.
    Maximum Number of Points: enter number greater than
 num. of particles
    Click (Apply) button
  In Display:
    Color by: Solid Color
    Change color if necessary
-- Display velocity/rotation vectors as colored arrows
Pipeline Browser: Click on Particles.00*
Main Menu: [Filters]->[Recent]->[Gliph]
Object Inspector:
  In Properties:
    Vectors:  Velocities [or RotationRates]
    Glyph Type: Arrows
    Scale Mode: vector
    Set Scale Factor:  change if necessary
    Maximum Number of Points: enter number greater than num. of particles
    Click (Apply) button
  In Display:
    Color by: Velocities      Magnitude
    Press (Edit Color Map ...)
      (Choose Preset) select one of the preset color scales
```

Of course, it is possible to paint particles according to a number of scalar quantities, such as `vx, vy, vz, |v|, wx, wy, wz, |w|`, etc.

```
Main Menu: [File]->[Open]  Select files Particles.00*
Pipeline Browser: Click on Particles.00*
Object Inspector: (Properties) (Apply)
--  Display particles as painted spheres
Main Menu: [Filters]->[Recent]->[Gliph]
Object Inspector:
  In Properties:
    Glyph Type: Sphere
    Scale Mode: scalar
    Set Scale Factor: check Edit box and enter 1.
    Radius: 1.
    Maximum Number of Points: enter number greater than num. of particles
    Click (Apply) button
  In Display:
    Color by: choose one of the variables
    Click (Edit Color Map) button
    Click (Choose Preset) button in color scale editor window
    Choose one of the color sheme and press the (OK) button
```

The following example shows the commands for generating a Paraview file which contains the exploded view of a particle list depicting the domain decomposition. The parameter 1.3 controls the amount of radial motion for the domains. The coordinates of the center of gravity of each domain are multiplied by this parameter. A value of 1. means all particles stay where they are. The larger the value of this parameter, the more 'exploded' the view looks. Results are in file `DomainDecomposition.000.vtu`. The domains may be painted using the scalar variable 'Domains'.

```
PlotList DomainDecomposition {
  Paraview
  TimeInterval 100. s
  ndL Particles {
    DomainDecomposition 1.3
  }
}
```

6.1.8 Nodal Rotations

For all finite element and discrete particle formulation in MARS is currently sufficient to keep track of rotation rates. Actual rotations, the change in orientation of the nodes or particles, are not used because most formulations employ an incremental approach for computing stresses and forces. There are situations where an analyst needs to process node-particle rotations. To satisfy this requirement, we have inserted in MARS the capability of keeping track of particle rotations, by introducing a new class (NodeQ) derived from class Node and class Quaternion. Class Node is used to instantiate all nodes and particles for most models. Class Quaternion implements quaternions, a mathematical construct which can be viewed as an extension of complex numbers. Quaternions are used to describe rotations in space employing only four scalars. A node list can be forced to use the NodeQ class rather than the default Node class by entering the keyword `ComputeRotations` in a stand-alone line

```
NodeList Particles {
  . . .
  ComputeRotations
  . . .
}
```

At this time, node rotations can only be viewed using Paraview. It is sufficient to enter a PlotList section in the input file using the following commands

```
PlotList Particles {
  TimeInterval 0.2 ns
  Paraview
  ndL Particles { }
}
```

Node rotations are automatically saved to the output plot-file along with coordinates, velocities, and rotation rates.

The new NodeQ class was tested on a simple benchmark problem consisting of a simple supported beam loaded with a uniform load perpendicular to the beam. The beam was modeled using a strip of quadrilateral shell elements. Vibrations were dampened until the steady state solution was obtained. The final rotation of the beam are visualized in Paraview using the steps described below

```
Load particle file ... [Apply]
(Main Menu) Filters -> Recent -> Gliph
- Set Gliph parameters in the [Properties] tab
  Scalars: Rotations
  Vectors: RotatiionVectors
  GlyphType: Arrow
Set Scale Factor: set to appropriate value by trial and error   [X] Edit
- Change color convention in the [Display] tab
  (Edit Color Map ...) -> (Choose Preset)
       Choose Red-Yellow-Green-Blue bar
```

If you want to show the particles as well, you must re-enter

```
Load particle file ... [Apply]
(Main Menu) Filters -> Recent -> Gliph
- Set Gliph parameters in the [Properties] tab
  Scalars: Rotations
  Vectos: RotationVectors
  GlyphType: Sphere
  Set node radii or scale particle radii as necessary
- Change color convention in the [Display] tab
  (Edit Color Map ...) -> (Choose Preset)
         Choose Red-Yellow-Green-Blue bar
```

6.1.9 Extract Commands

```
Extract Dogbone {
  Cyl // or Flat
  MinRad 6 cm  // throat
  MaxRad 8 cm  // base
  TotalLength 10 cm
  ThroatLenth 6 cm
}
```

6.1.10 Insert Commands

```
Insert LenticularFlaw {
  Center 5.6 nm 56. nm 64 nm
```

```
    X-Axis   1.3 4.5 2.4
    Y-Axis  3.4 6.7 8.4
    [ Thickness 5 nm ]
    X-Length 50 nm
    Y-Length 20 nm
    Plot
  }
  Insert Particles {
    Box { 10 cm 10 cm 5 cm }    GaussianRadiusDist { }
    Seed 345
    // either Number or UntilFull
    Number 200
    UntilFull
  }
```

6.1.11 Discrete Element Commands

```
Read DEM Particle File generated using John Peter's code
ControlParameters {
  Units Nano
}
NodeList Particles {
  Particles
  Density 2. g/cm3
  LengthUnits nm
  ReadDemParticleFile Problem3_RS_Final.pts
}
```

6.2 MacroParticle Lists

Macroparticles are assemblies of 3 or more spherical particles tied together either using rigid constraints or spring and dampers. ...

```
MacroParticleList 'ListName' 'Type' {
  // for available 'Types' see below
  Density 2.0 g/cm3
  // 1. Enter type dependent parameters (see below)
  Parameters { ... }
  // 2.a Generate one of the listed distributions
  Generate {
    Prism {
      X-first 0. in  X-inc 2. in X-rows 10
      Y-first 0. in  Y-inc 2. in Y-rows 10
      Z-first 0. in  Z-inc 2. in Z-rows 10
    }
```

```
    Cylinder {
      Center 0. in 0. in 0. in
      Radius 4. in
      Length 8. in
    }
    Sector {
      // x>0  y>0  0<z<L   r<R
      Radius 4. in
      Length 8. in
    }
  }
  // 2.b Read spheres from node list
  NodeList 'ListName'
  InsertNodeList ['ListName'] {
    . . .
  // Optional commands
  RandomRotations // (Opt.)
  Set vz -100 m/s // (Opt.)
  ReadPlotFile 'filename'
}
```

6.2.1 Flex 4-Sphere MacroParticle

```
MacroParticleList 'ListName' Flex4SphereParticle {
  . . .
  Parameters {
    SphereRadius
    TetRadius
    Stiffness
    Mom
    Vis
  }
}
```

6.2.2 Rigid 4-Sphere MacroParticle

Each macroparticle consists of an assembly of four spherical particles placed at the vertices of a tetrahedron and rigidly tied together

```
MacroParticleList 'ListName' Rigid4SphereParticle {
  . . .
  Parameters {
    SphereRadius
    TetRadius
  }
}
```

6.2.3 Rigid 3-Sphere MacroParticle

Each macroparticle consists of an assembly of three spherical particles placed at the vertices of a triangle and rigidly tied together

```
MacroParticleList 'ListName' Rigid3SphereParticle {
  . . .
  Parameters {
    SphereRadius 3. mm
    TetRadius 2. mm
  }
}
```

7 Edge/Truss/Beam Elements

7.1 Edge List

Edge lists are collections of 'edge' type objects. In its simplest geometric form, an edge is a line segment spatially defined by two nodes. MARS implements edges in an 'Edge' class. Several structural entities can be derived from the edge class: trusses, rebars, beams, links, etc. Edge lists can be created internally from other lists or input explicitly. When created from other lists, they are typically used in conjunction with more complex meshes consisting of triangular and quadrilateral faces or tet and hex solids. Input commands for defining new lists explicitly via input are given below. below.

```
EdgeList 'EdgeListName' 'type' {
  // where 'type' can be one of the following
  // Geometry
  // Truss
  // Rebar
  // 'EdgeList Edges {' with no specifier defaults to Geometry
  // ** 1. ** Specify node list
  NodeList 'NodeListName'
  // or
  InsertNodeList 'NodeListName' { . . . }
  // ** 2. ** Read or generate edges
  ReadObjects 345
  //  i   n1   n2
      1  124  243
      2   56  238
      . . .
  // else
  Generate {
  // see below for generation options
  }
```

```
  // ** 3. ** Change attributes (optional)
  Color Green
  Radius 0.4 mm     // [1]
  Diameter 0.8 mm   // [1]
  Density 7.8 g/cm3 // [2]
  PlotAttributes {
    Cylinders
  }
  // ** 4. ** Other optional commands
  EditNodeList { . . . }
  Make EdgeList 'SubListName' // sublist of selected edges
  Make NodeList 'SubListName' // nodes attached to selected edges
  // select, unselect, alsoselect commands see below
  // writing and reading external files
  Write PartMeshDataFile PART.mrs // [3]
  Read PART.mrs  // [3]
}
```

[1] The radius or diameter are used for three main purposes: a) plot edges as three-dimensional cylinders, b) provide a radius for edge-edge contacts, c) compute masses for rigid body applications.
[2] Density is used for computing nodal masses when an edge list is used in the definition of a rigid body.
[3] The `Write PartMeshDataFile` command creates an ASCII file with node and edge information with this format:

```
// commented title line
  InsertNodeList 'listName' {
    LengthUnits in
    ReadNodes 235
    . . . // nodal coordinates
  }
  ReadObjects 211
  . . .  // edge indeces
EOF
```

The mesh data can be used as input to other files using the `Read PART.mrs` command

When generated from other lists, it is possible to change some list attributes, like color, as shown in this example:

```
QuadFaceList 'ListName' {
  . . .
  Make EdgeList 'EdgeListName' SharpEdges
}
EdgeList 'EdgeListName' {
  Color Red
}
```

7.1.1 Generate commands

The generate commands are shared with beam lists. Multiple parts or lines can be generated within the same block of instructions:

```
  Generate {
    StraightLine { ... }
    StraightLine { ... }
    Helicoid { ... }
  }
```

The overlapping nodes from these diferenct parts can be merged using the MergeNodes command.

Straight Line

```
    StraightLine {
      LengthUnits cm
      FirstPoint 0.0 0.0 0.
      LastPoint 20. 0.0 0.
      // you can also enter first and last node provided you entered a node list
      FirstNode 1
      LastNode 2
      NumberOfSegments 10
    }

BeamList RBRS {
  sec o m STEL #3
  Generate {
    Rebars {
      ReferenceSystem RSYS
      // rebars are aligned in RSYS-X direction
      LengthUnits cm // required
      Translate 0. 0. 5. // in global RefSys, optional
      RebarLength 10.
      MaxElementSize 2.
      NumberOfRebars 6  // optional, dfl = 1
      RebarSpacing 4. // in local Y direction
  }
}
EdgeList RBRS Rebar {
  Material Steel
  Size #3
  Generate {
    Rebars {
      ReferenceSystem Local
```

```
      // rebars are aligned in Local-X direction
      LengthUnits cm // required
      Translate 0. 0. 5. // in global RefSys, optional
      RebarLength 10.
      MaxElementSize 2.
      NumberOfRebars 6  // optional, dfl = 1
      RebarSpacing 4. // in local Y direction
    }
    BentRebars {
      ReferenceSystem Local2
      LengthUnits in
      MaxElementSize 1.
      Translate 0. 0. 5.    //
      Point 0. 12. -35  // 1st point
      Point 0. 15. -35  // 2nd point
      Point 0. 15. -30  // 3rd point
      [ CloseCurve ]
      Duplicate 5 @ 10.
    }
  }
}
```

Parallel fibers

This scheme generates a system of straight parallel fibers aligned in the z-direction. The whole system is centered at the origin but can be later translated and reoriented. The fibers are equally spaced in the x- and y-direction. The pitch as well as the number of fibers in the x- and y-directions are independently defined. The number of fibers in each direction should be an odd number so that there are an equal number of fibers before and after the middle fiber, the fiber that crosses the origin. The input commands are given below

```
EdgeList 'ListName' Geometry {
  Generate {
    ParallelFibers {
      Length 2. in
      X-Pitch 0.25 in
      X-Fibers 51
      Y-Pitch 0.25 in
      Y-Fibers 51
    }
  }
}
```

The fibers can be translated and reoriented in any direction using the move and rotation commands for node coordinates. For example, if the fibers need to be aligned with the

y-direction, we need to rotate all nodes by 90 degree around the x-axis. Tthe sequence of transformations (rotations and translations) matters as they are done in a sequential order.

```
EdgeList 'ListName' Geometry {
  Generate {
    ParallelFibers {
    . . .
    }
    EditNodeList {
      X-Rotate 90 deg
      Move 0. in  0. in 1. in
    }
  }
}
```

When the system of parallel fibers is embedded in a LDPM solid, the portions of fiber sticking out of the solid can be chopped.

Parallele wires

This features was inserted for generating models of cable used in suspension bridges

```
BeamList CABL {
  sec o m STEL r 0.1
  Ref CABL
  Generate {
    generate a bundle of wires inside a 10 in circle
    Bundle L 12. l 1. d 0.2 R 10. o S CYLN
  }
}
```

Helicoidal wire

```
BeamList HLCD {
   sec o m STEL r 0.1
   Ref CYLN
   Generate {
     Helicoid R 10. L 0.2 n 60. L 10  S CYLN q
  }
}
```

Random fibers

```
EdgeList FBRS Truss {
  Generate {
```

```
    RandomFibers {
      Volume -6 in 6 in -6 in 6 in -0.25 in 0.25 in
      Length 5 cm
      ElementSize 1 cm
      Seed 134
      // increase Bending to make fibers more contorted
      Bending 0.9
      NumberOfFibers 2000
    }
  }
```

Twisted Cable

This generation scheme generates straight segments of twisted cable. The input parameters are shown below. The best way to test this generation scheme is to start from the input below, ake changes to the input and visually display the resulting mesh. In a twisted cable, individual wires are kept from crossing each other using the edge-edge contact algorithm. The node-edge contact algorithm may be sufficient for some simulations, saving time but being potentially unreliable.

```
BeamList CABL {
  sec o m STEL r 0.1 in
  Generate {
    TwistedCable {
      Strands 7 // 1, 7, or 19
      WiresPerStrand 7 // 1, 7, or 19
      WireRadius 0.1 in
      CableLength 100. in
      ElementLength 2. in
      WireRotationPitch 10.
      StrandRotationPitch 20.
    }
  }
}
```

7.1.2 Select commands

The edge select commands make is possible to select a subset of edges using various criteria. The selection can be saved in a separate list using the `MakeList` command or used on a temporary basis. The standard `Select` commands are available:

```
Select [criterion]
AlsoSelect [criterion]
Unselect [criterion]
Reselect [criterion]
InvertSelection
```

Selection criteria, `criterion`, can take any of the the following forms

```
all    // all elements
do 25  // element 25
do 1 5 // elements 1 through 5
do 1 100 2 // elements 1 through 100 step 2
cp 0. 0. 1. > 0.4  // elemenst such that cross product with
    // vector 0,0,1 is greater than 0.4
1n // elements with at least one node selected
2n // elements with both nodes selected
Example:
  Select do 1 100 // select element 1 through 100
  AlsoSelect do 201 300 // add elements 201 - 300
```

In addition, three separated commands ara available to select, unselect, or reselect nodes which are used in the definitions of the selected edges in the list: `SelectNodes`, `UnselectNodes`, and `ReselectNodes`. For example, the commands below are used to select the nodes of the first forty edge elements in the list.

```
EdgeList 'listName' Geometry {
  . . .
  Select do 1 40
  SelectNodes
}
```

These commands are also applied to all other types of lists which are derived from the edge list.

7.1.3 Make commands

The `Make EdgeList` command is used for generating a sub-list of edges which have been previously selected. The new list is of the 'Geometric' type; in other word, MARS will not perform any operation on it (e.g. computer internal forces).

The `Make NodeList` command is used for generating a sub-list of nodes which are used for defining the edges in the current edge list.

7.1.4 Notes

Currently, beam elements, although derived from the 'Edge' class, are treated in a separate list called 'BeamList'. This may change in future versions of MARS. MARS.

The command 'Write PartMeshDataFile' and 'ReadFile' can be used to transfer mesh details to a separate file and clean up the main input file. For example, we may import a truss edge mesh generated using a processor code and convert it to MARS; in the conversion run, the edge list can be saved using the command

```
Write PartMeshDataFile PART.mrs
```

In the main input file, the edge data can be loaded using the commands commands

```
EdgeList 'ListName' 'type' {
  Read PART.mrs
}
```

Note that the mesh part file includes the edge definition as well as the node data. Sections 1. and 2. of the edge list input should not be present in the main input file. file.

7.1.5 Linear Elastic Beams - Uniform Cross Section

This list consists of a collection of linear elastic beams with uniform cross section. The beam formulation is based on the Euler-Bernoulli beam theory. A beam element is defined using two nodes. Each beam element has a corotational local reference system XYZ. The X direction is aligned with the beam axis from node 1 to node 2. The second Y direction is perpendicular to X and is initialized at time zero using a `ReferenceSystem` object previously defined. The section properties are defined in the local Y-Z plane perpendicular to the beam axis. The sections properties consists of the following data:

- cross section area `A`,
- moment of inertia about the Y-axis `IY`,
- moment of inertia about the Z-axis `IZ`, and
- torsion constant `J`.

The torsion constant of the section is not to be confused with the polar moment of inertia. The two are identical for round shafts and concentric tubes only. For other shapes `J` must be determined by other means. The section properties are internally calculated for a few common cross sections (see sample input listing below) or explicitely entered.

```
EdgeList 'listName' LinearBeam {
  Material 'materialName'
  // Select one of the available cross sections
  RectangularCS { by 3. in  bz 0.5 in }
  CircularCS { Ro 5.125 in  Ri 4.875 in }
  // or specify cross section properties explicitely
  CrossSection { A 4in2  IX 5.33 in4 IY 0.33 in4  J 5.1 in4 }
 // Read mesh
  NodeList 'nodeListName'
  ReadObjects 1
  //j  j1 j2
    1   1  2
  // or generate mesh internally
  Generate {
    // see generate commands for EdgeList
  }
}
```

7.1.6 Linear Elastic Beams - Non-Uniform Cross Section

This list is essentially an extension of the previous list. The only difference is that, as the name implies, the cross section properties may vary from beam to beam. Thus, the input line for each beam must include the definition of the section properties explicitely, as shown in the example below. below.

```
EdgeList 'listName' LinearBeamNonUniformCS {
  NodeList 'nodeListName'
  Material 'materialName'
  ReferenceSystem 'refSysName'
  ReadObjects 10
  // j n1 n2  other data
     1  1  2  L in  Y 0. 1. 0.  A 2.17  IY 1.8  IZ 1.8  J 3.601
     2  2  3  L cm  n3 9  A 3.763  IY 2.813  IZ 2.813  J 5.626
     3  3  4  Rect { bY 2.125 in  bZ 1.5 in }
     4  4  5  Rect { b 2.125 in }
     5  6  6  Circ { Ro 4 in }
     6  6  7  Circ { Ro 4 in Ri 3.5 in }
     7  7  8  I { wf 2. in  tf .2 in hw 2. in tw 0.1 in }
     . . .
}
```

For the first beam, the cross section properties are entered explicitely. In this case, it is mandatory to enter the length units, `L in`. The local Y-direction is entered specifying a vector V using the command(`Y 0.  1.  0`). The vector V does not need to be unitary or perpendicular to X. The local reference system is computed using these operations: Z = X x V, and Y = Z x X, where 'x' is the vector outer product.

For the second beam, the Y-direction is specified using a third node `n3`. In this case, the Y-direction is oriented from the projection point of `n3` on the beam toward node `n3` itself.

For the third beam, the cross section is rectangular with 2.125 in in the local Y-directions and 1.5 in in the Z-direction. Square cross sections can be also specified as in the fourth beam.

For the fifth beam, the cross section is a solid cylindrical rod with radius 4. in. Annular cross sections can be specified as in the sixth beam.

7.1.7 Plotting options

The plotting options are used for choosing three dimensional rendering shapes in Quasar. Note that special shapes can be done in Paraview using gliphs objects. These shapes are available, `Cylinders`, `HiResCylinders`, and `Pills`. Any one of these shapes can be specified in this fashion,

```
EdgeList 'listName' Geometry {
  . . .
```

```
  PlotAttributes {
    // Select only one
    Cylinders
    HiResCylinders
    Pills
  }
}
```

The `Pills` option is used to render each segment in the shape of a pill, that is a cylindrical portion with two hemispherical caps. The diameter of the 'pill' is entered using the `Radius` command in the regular section of the input.

When `Cylinders` or `HiResCylinders` is used in Paraview, the data is written in a special format so that the rendering is done in Paraview using glyphs. These are the steps in Paraview for rendering the data:

1. Open plot files corresponding to edge list
2. Press 'Apply' button (nothing shows up)
3. Select 'Filters' - 'Common' - 'Glyph' from main menu
4. Set 'GlyphType' to 'Cylinder'
5. Set 'Resolution' value to 30 or higher
6. Set 'Radius' value to desired value
7. Leave 'Capping' checked
8. Set the 'Glyph Transform' 'Rotate' value to (0, 0, 90)
9. Set 'Scale Mode' to 'scalar'
10. Check 'Edit' and set 'Set Scale Factor' to 1. or slightly higher
11. Press 'Apply' button (the cylinders should show up)
12. In the Display tab, change 'Color by' to 'Solid Color'

Step 8 is necessary to have the cylinder aligned with the direction of the edge. This may be corrected in newer versions of Paraview and this step may no longer be necessary.

Steps 9 and 10 are intended to scale the height of the cylinder to the length of the edges. If the edges form a curved line, it is necessary to use a value greater than 1. to avoid gaps on the convex side of the line.

7.2 Beam Lists

The BeamList is used to define a set of beam elements with constant cross section. The formulation is similar to the QPH shell element, in the sense that the centerline of a beam element remains straight. Shear deformations are controlled by the rotation rates of the two nodes that define a beam. The beam formulation has a modular interface with the CrossSection object. This makes it possible to define many types of cross-section integration schemes and easily add new ones.

```
BeamList Rebars {
  // 1) RefSys is used to set beam 2nd direction
  ReferenceSystem 'RefSysName' // {1}
```

```
  // 2) select one of the cross section types
  sec o { }  // solid cylindrical cross-section
  sec O { }  // tubular cross section
  set h { }  // hat section
  sec I { }
  sec R { }  // rectang hollow cross section
  sec Z { }  // Z section
  sec c { }  // custom section
  // 3.1) specify mesh explicitely
  NodeList Nodes
  ReadObjects 345 // number of elements
  //  i   n1   n2
      1  124  243
      2   56  238
      . . .
  // 3.2) else generate mesh
  generate {
    // see below for mesh generation options
  }
  // 3.3) else read mesh from external file
  ReadFile 'filename' // optional
  Read PART.mrs
  // 4) specify plot attributes
  Color Rust
  // 5) writing and reading external files
  Write PartMeshDataFile PART.mrs
}
```

[1] The selection of the reference system is very important specially for cross sections that are not axi-symmetric. The provided reference system is used for setting up the local co-rotational reference system for each beam element during the initialization phase. The local x-axis is oriented in the direction of N1 to N2 where N1 and N2 are the two nodes defining the beam element. The specified reference system returns a preferential direction at each point in space [see section describing reference systems]. During beam initialization, the preferential direction U is computed at the beam midpoint. This makes it possible to compute the Z direction of the local z-axis as a outer product Z = X x U. The Y direction is then computed as Y = Z x X. The best way to check that all beam have been initialized properly is to plot them.

7.2.1 Time History Commands

Currently, it is possible to save the total axial force in a single beam element and material state variables at an integration point of an element. In the example below, we request the axial force of element 23 and the state variable number 2 (one of the shear stresses) of the element whose centerpoint is closes to a point with coordiates 0.1, 0.5, 0.3 in inches.

```
TimeHistoryList Hist {
  . . .
  bm-Rebars 23 af  // axial force
  bm-Rebars cl 0.1 in 0.5 in 0.3 in  ip 1 sv 2
}
```

In the future, it would be desirable to also be able to compute the maximum bending moment in an element.

7.2.2 Plot Commands

Plotting attributes can be specified in the element list or in the plot list

```
BeamList PART {
  . . .
  PlotAttributes {
    ContourVariable sv 1
    NoNodalAveraging
    NoSmoothing
    HighResolution
    MediumResolution
  }
}
PlotList PLOT {
  . . .
  bmL PRT1 {
    // you may selecte one of the contour variables below
    ContourVariable StateVariable 1
    ContourVariable Velocity
    ContourVariable X-Velocity
    ContourVariable Y-Velocity
    ContourVariable Z-Velocity
    ContourVariable AxialStretch
    // stresses are averaged at the nodes unless ..
    NoNodalAveraging
    NoSmoothing  // discrete colored fringe plots
    // prescribe range after countour variables is selected  (use appropriate units)
    RangeMinValue 0 psi
    RangeMaxValue 10000 psi
  }
}
```

Fragmentation Commands

The beam fragmentation scheme is consistent with the fragmentation schemes employed for quadrilateral and hexahedral meshes. Failed elements are not 'eroded' or 'nullified'

as in other common schemes. Instead, elements are disconnected at their common node when local failure criteria are satisfied. This is accomplished by inserting a new node and performing a local remeshing by indroducing a discontinuity in the mesh. A temporary cohesive element is introduced between the two overlapping nodes for dissipating fracture energy. Currently, the failure criterion at the node that connects to adjacent elements is based on the average stretch of the two elements. When the average stretch exceeds an input failure value, then the two elements are disconnected. It is possible to introduce stochastic failure by assigning a statistical distribution to the allowable stretches at the nodes. In this case, the failure stretch for each node is computed at the beginning of the simulation by multiplying the input failure stretch ing a parameter obtained from the requested statistical distribution. In this fashion, some spots are weaker than others.

```
#-- Add following lines after element definition
  Weibull { . . .  } // optional statistical distribution
  Cracking { fail 0.03  [ decay 0.8 ] [ stiff 3 ] }
  // fail 0.03 : failure stretch, [1]
  // decay 0.8 : insert penalty spring and reduce force [2]
  // stiff 3:  do not fail 3 bonds adjacent to failed bond [3]
```

[1] Failure stretch has no dimensional units. Two beam elements are disconnected at their common node when the average stretch of the two elements exceeds the local failure stretch at the node.
[2] The `decay` parameter is used to reduce the cohesive force as the two elements are pulling apart from each other, thus dissipating a certain amount of energy (fracture energy).
[3] The `stiff` parameter is used to prevent a string of elements from fracturing into single element fragments.

Square solid section

```
  sec s m MATE r 10 mm i 5 p 4
  m: material
  s: side , can also use
         A 315 mm2 // section area
  i: # of int points =6,  2x2 truss points + 2 shears
                     =11, 3x3 truss points + 2 shear
  p: # of plotting pnts =0: line
                        =4: square
```

Circular solid section

```
  sec o m MATE r 10 mm i 5 p 1
  m: material
  r: radius, can also use
         d 20 mm // diameter
         A 315 mm2 // section area
```

```
i: # of int points =1 truss
                   =5 beam with 3 tensile IP
p: # of plotting pnts =0: line
                      =1: cylinder
                      =6: hexagonal X section
                      =12: 12 sided X section
```

Tubular section

```
sec O m 'MaterialName' r 10 mm t 1 mm i 5 p 1
m: material
r: radius, can also use
       d 20 mm // diameter
t: thichness
i: # of int points around circumference
p: # of plotting pnts =0: line
                      =1: cylinder
                      =6: hexagonal X section
                      =12: 12 sided X section
```

Z section

```
sec O m MATE t 1 mm h 10 mm w 10 mm
m: material
t: thickness
h: height
w: width
x: x-offset
y: y-offset
```

Hat section

```
*---*     *---*
  a |h    | a     y
    |  b  |       |
    *--o--*       +--x
sec h m MATE  t 1  h 10  W 15  a 4
m: material
t: thickness
h: height
a: flange width
b: flange width
W: total width (W = a+b+a)
x: x-offset
y: y-offset
```

7.3 Geometric Pair Detection

The node-pair lists consist of a set of lists that implement various types of interactions between two nodes or two particles (recall that in MARS particles and nodes are used interchangeably). Note that this set includes a master-slave formulation, which is a type of constraint list, but not the inter-particle contact list, which is grouped with the contact lists.

7.4 Geometric Pair-Detection

```
NodePairList 'ListName' Geometry {
  NodeList 'List1Name'
  NodeList 'List2Name'
  DetectionDistance 0.6 cm
  Node1Thickness 0.4 cm
  Node2Thickness 0.2 cm
}
```

7.5 Master-Slave Constraints

This list consists of a set of master-slave constraints between pairs of nodes. The constraint formulation makes it possible to release some degrees of freedom with respect to a local co-rotational reference system which rotates along with the master node. Each constraint is defined in a single input line. The input consists of two nodes, the first node is the master node, the second node is the slave node. The nodes can be in the same list or different lists. No requirement is made on whether the nodes are overlapped. If nothing else is specified, then all six degrees of freedom are tied. If some DoF's need to be released, then an initial local reference system need to be defined.

```
NodePairList 'ListName' MasterSlaveConstraints {
  ReadObjects 2
    // 1st node is master, 2nd node is slave like in master-slave
    'NodeListName'-34 'NodeListName'-43 L 'RefSysName' T XXX R OXX
    'NodeListName'-14 'NodeListName'-76 X 0.7 0.7 0. Y 0. 1. 0. R XOX
}
```

For example, to model a hinge around the local X axis it is necessary to specify a local reference system which includes the X axis (as well as a Y axis which can be any arbitrary direction perpendicular to the X axis), and the `R OXX` labels. A spherical bushing can be specified by entering the label `R OOO` only.

7.6 Node-Pair Attraction List

```
NodePairList PosNegPairs Attraction {
  NodeList PosNodes
  NodeList NegNodes
```

```
  DetectionDistance 0.6 cm
  Node1Thickness 0.4 cm
  Node2Thickness 0.2 cm
  AttractionConstant 45
}
```

7.7 Node-Pair Repulsion List

```
NodePairList PosNegPairs Repulsion {
  NodeList PosNodes
  DetectionDistance 0.6 cm
  Node1Thickness 0.4 cm
  RepulsionConstant 45
}
```

7.8 Node-Pair VanDerWaals List

```
NodePairList 'AttractionForces' VanDerWaals {
  NodeList 'Particles'
  DetectionDistance 4 cm
  NodeThickness 0.4 cm
  HamakerConstant 45
  ThreshholdGap 0.4 nm
}
```

7.9 Node-Pair NanoParticle List

```
NodePairList 'ListName' NanoParticles {
  NodeList 'Particles'
  DetectionDistance 4 cm
  NodeThickness 0.4 cm
  UpdateInterval 1. ns
  ContactForce Hertz {
    YoungsModulus 59 MPa
    PoissonsRatio 0.2
  }
  FrictionForce {
    StaticFriction 0.3
    DynamicFriction 0.2
  }
  RollingResistance {
    Kr 1.e-4  Kt 1.e-4 Fr 0.2 Ft 0.2
  }
  VanDerWaalsForces {
    HamakerConstant 1.61e-20 J
```

```
    ThreshholdGap 0.4 nm
  }
  IonicForces {
    DLVO // or SI
  }
}
```

7.10 Nano Particles

The nano-particle interaction list employs the same contact models which are used in the contact list. Please, refer to the 'contact models' section of this manual.

A minor difference between regular contact between particles and contact formulas for nano-particles is the way nano-particle penetration is calculated. The acutal gap between two nano-particles is calculated using the formula:

$$g = d - r_1 = r_2$$

where d is the distance between the centers of the two particles, r_1 and r_2 are the radii of the two particles. For contact purposes, the gap can be redifined by controlling the range of the particle radii, [rmn-rmx]. Essentially, particle radii must be at least rmn but no more than rmx, as shown in this code snippet:

```
R1 = max(rd1, rmn);
R1 = min(R1, rmx);
R2 = max(rd2, rmn);
R2 = min(R2, rmx);
gapC = dst - R1 - R2;
```

The negative of 'gapC' is the inter-particle penetration which, when positive, is used to compute contact forces. The values of rmn and rmx are initialized to 0. and 1.e30 respectively. They are specified via input using the commands:

```
MinContactRadius 4 nm
MaxContactRadius 8 nm
```

If the user wants to set the radii of all particles to the same value, the following command

```
ContactRadius 5 nm
```

sets rmn = rmx = 5 nm. nm.

7.10.1 Tabulated Forces

When the built-in equations are not adequate for representing the inter-particle forces, including ionic forces, it may be desirable to define these forces as a tabulated function, where x is the the inter-particle gap and y is the inter-particle force. Note that these forces overlap to any other force, including contact and VanDerWaals forces.

```
LoadCurve 'CurveName' {
  // inter-particle force versus gap table
  . . .
}
NodePairList 'ListName' NanoParticles
  . . .
  TabulatedForce 'CurveName'
}
```

7.10.2 VanDerWaals Forces

The VanDerWaals force is the attractive or repulsive force between molecules (or between parts of the same molecule) other than those due to covalent bonds or to the electrostatic interaction of ions with one another or with neutral molecules [Wikipedia]. The expression for the VanDerWaal force implemented in MARS employs the Hamaker constant 'hmk' and a treshold gap value 'thg'. The C++ code of the implementation is listed below.

```
  D = 2. * min(R1, R2); // R1, R2 radii of the two particles
  gp = max(wgp, thg);  // wgp: gap between the two particles
  x = gp / D;
  x1 = x + 1.;
  x2 = x * (x+2.);
  // expression for the VanDerWaals force 'frc'
  frc = hmk/(6.*D) * (2.*x1/x2 - x1/(x2*x2) -
                      2./x1 - 1./(x1*x1*x1));
```

The input for VanDerWaals forces is shown below

```
NodePairList 'ListName' NanoParticles
  . . .
  VanDerWaalsForces {
    HamakerConstant 1.61e-20 J
    ThreshholdGap 0.4 nm
  }
```

7.10.3 Plotting Options

It is possible to generate contour plots of the contact stresses. Contact stresses are computed as described in the online manual. The command for generating contour plots in Quasar format are given below.

```
PlotList 'ListName' {
  . . .
  npL 'ListName' {
    RedValue -100 psi
```

```
    BlueValue 0 psi
    StressComponent XX
    // valid components are: XX, YY, ZZ, YZ, ZX, XY
  }
}
```

If the Paraview format is chosen, then, there is no need to specify stress components and min-max values. These operations are done in Paraview. The Paraview file contains eight records listed below:

```
  1. XX-component of the contact stress
  2. YY-component of the contact stress
  3. ZZ-component of the contact stress
  4. YZ-component of the contact stress
  5. ZX-component of the contact stress
  6. XY-component of the contact stress
  7. Maximum contact stress
  8. Force chain vector
```

Note that Paraview makes it possible to plot force chain vectors. The commands for writing a Paraview file sequence are:

```
PlotList 'ListName' {
  Paraview
  . . .
  npL 'ListName' { }
}
```

7.11 Node-Pair Penalty Constraints

```
NodePairList 'ListName' PenaltyConstraints {
  ForcePenaltyStiffness 1.e N/m
  // use MomentPenaltyStiffness to constrain moments
  [ MomentPenaltyStiffness 1.e Nm ]
  ReadObjects 2
    'List1'-34 'List2'-43
    'List1'-14 'List2'-76
}
```

8 Triangular Faces and Shell Elements

8.1 Triangular Face Lists

The TriangFaceList is used to define a set of triangular faces. These faces can represent:

- purely geometric entities,

- faces subjected to pressure,
- membrane elements,
- shell elements,
- a set of disconnected rigid triangles.

The type of face is specified in the first line after the list name. The most basic list is the geometric type, where objects consists of triangular faces defined by three nodes. The commands below refer to geometric lists but can also be used in the other lists. Other lists have additional commands which are described in later sections. Note that the triangular face lists created by other lists, e.g. the external faces of a tetrahedral mesh, are of the geometric type.

```
TriangFaceList 'ListName' 'type' {
  // where the keyword 'type' can be one of the following:
  // Geometry: this can be used to define plain faces
  // Rigid: this is used to define rigid triangular platelets
  // UniformPressure: surfaces subjected to pressure loads
  // MultiplePressureHistories:
  // DktShell:
  //
  // 1. Specify thickness [Optional]
  Thickness 0.125 in  // default = 0.
  // 2. Specify density for rigid body calcs [Optional]
  Density 7.8 g/cm3
  // if thickness = 0, then mass is also 0.
  // 3. Specify front and/or back color [Optional]
  FrontFaceColor gray // default  lightgray
  BackFaceColor red // default  lightgray
  // 4. Specify node list
  NodeList NODS
  ReadObjects 254 // number of faces
  //  i   n1   n2   n3
      1  124  243   56
      2   56  238  121
      . . .
  // select commands
  Select, Unselect, ... // see below
  // make commands
  Make TriangFaceList Sublist // list of selected faces
  Make EdgeList SharpEdges //  see below
  Make NodeList SelNodes // list of nodes attached to selected faces
  SelectNodes // attached to selected faces
  // face orientation command
```

```
  InvertOrientation // invert orientation of all faces
  // orient faces so that normal is toward direction nx, ny, nz
  Orient Direction nx ny nz
  // orient faces so that normal points toward point
  Orient Toward 1. cm 5. cm 3. cm
  // orient faces so that normal points away from point
  Orient AwayFrom 1. cm 5. cm 3. cm
  // orient faces in same orientation as face 56 using wavefront method
  Orient Wavefront 56
  Write PartMeshDataFile PRT1.mrs
  ReadFile PRT1.mrs
}
```

8.1.1 Select commands

```
Select [criteron]
AlsoSelect [criteron]
Unselect [criteron]
Reselect [criteron]
InvertSelection
[criterion] can take the following forms
all    // all faces
for 25  // face 25
for 1 5 // faces 1 through 5
for 1 100 2 // faces 1 through 100 step 2
FacesWithAtLeast1NodeSelected  //  in short: 1n
FacesWithAll3NodesSelected // in short: 3n
FacesPointingToward 0. 5. 4. // in short: tw 0. 5. 4
FacesWithCrossProduct 1. 0. 0. > 0.5 // in short: cp 1 ...
// faces such that cross-product with 1,0,0 is greater than 0.5
```

In addition, it is possible to select (or unselect) nodes attached to the faces that are selected using the commands `SelectNodes` and `UnselectNodes`. Examples are given in the selection section of the node lists

8.1.2 Generate commands

Several simple triangular meshes can be internally generated in MARS. Following is a list of surfaces that can be generated. Multiple surfaces can be generated withing the same 'Generate' block and merged together with the 'MergeNodes' command

```
  Generate {
    Cylinder {
      ReferenceSystem Local
      EdgesOnCircle 36 // must be multiple of 6
      Radius 4. in
```

```
    Length 10. in
    ElementSize 1. in  // in axial direction
  }
  Disk {
    ReferenceSystem Local // optional
    Radius 4. in
    OutsideEdges 36 // must be multiple of 6
  }
  Annulus {
    ReferenceSystem Local // optional
    InnerRadius 4. in
    OuterRadius 6. in
    InsideEdges 24 // must be multiple of 6
    OutsideEdges 36 // must be multiple of 6
  }
  Sphere {
    ReferenceSystem LOCL
    Radius 10. in
    Refinement 3
  }
  Single {  }
  Rectangle {
    1 10 ; 1 6 ; //  index progression like in INGRID
    -5. 5.       //
    -5. 5.       //
  }
  Box {
    Dimensions 2 m 2 m 5 m
    Elements 4 4 10
  }
GenericPlate { // [1]
  u in   // length units for this part
  R RSYS  // reference system [optional]
  L 0.15  // typical length of an element
  i  // invert quad orientation if necessary
  P // define polygonal external outline
  n 0.0 0.0  // first node of polygon
  n 1.0 0.0  // second node of polygon
  . . .
  c  // close the polygon
  //  enter internal circular holes (x, y, R)
  s 5  // min no. of sides in holes [optional]
  C 0.5 0.5 0.2 // [2]
  . . .
}
```

```
   MergeNodes 0.001 in // tol = 0.001 in
   }
}
```

[1] This command is used to generate a flat plate with an arbitrary polygonal outline containing any number of circular holes. The polygonal outer outline is defined entering the coordinates of the vertices of the polygon. This generation scheme employs the external program `triangle`.

[2] Enter one line for each hole. The format is `C xc yc rad`, where `xc` and `yc` are the coordinates of the center and `rad` is the radius. The hole should be fully contained inside the master polygonal surface.

8.1.3 Make commands

The `Make TriangFaceList` is used for generating a sub-list of triangular faces which have been previously selected. The new list is of the 'Geometric' type; in other word, MARS will not perform any operation on it (e.g. computer internal forces).

The `Make EdgeList` command is used to generate a list of edges from the edges of the triangular faces. This command must be terminated by a keyword for the edge selection criterion; three options are available:

```
Make EdgeList ListName AllEdges
Make EdgeList ListName SharpEdges
Make EdgeList ListName UnmatchedEdges
```

The option `AllEdges` is used to generate a list of all edges of the triangular mesh. The option 'SharpEdges' is used to generate a list of edges for which the attached faces form an angle greater than 60 degrees. The option `UnmatchedEdges` is used to generate a list of edges which are shared by a single face; note that if the surface is closed (e.g. a hollow prism), all edges are *matched* and the generated edge list will be empty. The list generated using the `SharpEdges` command includes unmatched edges.

8.1.4 How to make sublists

It is often desirable to make sublists from a parent list to isolate a set of faces on which we may want to impose special conditions. For example, let's consider a tetrahedral mesh of a solid cylinder. We want to create four lists:

1. top circular surface
2. bottom circular surface
3. top and bottom surfaces
4. cylindrical surface

The sublists may be used to impose independent pressure conditions. The commands for accomplishing this objective are shown below. For convenience, we assume that the cylinder is oriented in the z-direction and the coordinates of the bottom and top faces are respectively 0. in and 4. in.

```
TetSolidList Cylinder Geometry {
  . . .
  Make TriangFaceList CylinderFaces
}
TriangFaceList CylinderFaces {
  EditNodeList {
     Select cz > 3.99 in
  }
  Select FacesWithAll3NodesSelected
  Make TriangFaceList TopSurface
  EditNodeList {
     Select cz < 0.01 in
  }
  Select FacesWithAll3NodesSelected
  Make TriangFaceList BottomSurface
  EditNodeList {
     Select cz < 0.01 in
     AlsoSelect cz > 3.99 in
  }
  Select FacesWithAll3NodesSelected
  Make TriangFaceList TopBottomSurface
  InvertSelection
  Make TriangFaceList CylindricalSurface
}
```

A more compact way to accomplish the same task is shown below:

```
TriangFaceList CylinderFaces {
  Select FacesWithCrossProduct 0. 0. 1. > 0.5
  Make TriangFaceList TopSurface
  Select FacesWithCrossProduct 0. 0. -1. > 0.5
  Make TriangFaceList BottomSurface
  AlsoSelect FacesWithCrossProduct 0. 0. 1. > 0.5
  Make TriangFaceList TopBottomSurface
  InvertSelection
  Make TriangFaceList CylindricalSurface
}
```

In this cases the faces of the top surface are selected by using the criterion that the cross product of their normal with vector 0, 0, 1 is greater than 0.5. By using appropriately

the node selection and face selection commands, it should be possible to extract a list of faces that make up the desired surface. The sublist can be used to applied pressure loads as in the example below.

```
TriangFaceList CylinderFaces {
  Select FacesWithCrossProduct 0. 0. 1. > 0.5
  Make TriangFaceList TopSurface
  Select FacesWithCrossProduct 0. 0. -1. > 0.5
  Make TriangFaceList BottomSurface
  AlsoSelect FacesWithCrossProduct 0. 0. 1. > 0.5
  Make TriangFaceList TopBottomSurface
  InvertSelection
  Make TriangFaceList CylindricalSurface
}
```

It is a good idea to first run the problem in interactive mode and at the interactive prompt, select the lists and plot them to verify that the commands produced the desired surfaces.

8.2 Wet Triang Face List

These lists are used for applying pressure loadings on a set of triangular faces. Several loading types are available:

1. Uniform pressure loading
2. Variable pressure loading
3. Special loads
4. Patched pressure histories

The general syntax for these lists uses the format below. More details are given for each specific loading tpye.

```
TriangFaceList 'listName' 'loadingType' {
  . . .
}
```

8.2.1 Uniform Pressure

This list is used for prescribing a time-dependent uniform pressure history over a set of triangular faces. The pressure can be prescribed either using a 'LoadCurve' tabulated expression or using an 'Equation'. The latter is particularly useful when the pressures depend on the change in volume affected by the motion of the faces themselves. The single value time-dependent pressure is multiplied by the current area of each face in the direction opposite to its normal.

```
Equation 'equationName' {
  . . .
}
TriangFaceList 'ListName' MultiplePressureHistories {
    // 1.) Specify face list (Req.), either a face list
    //     or a shell list
    Link FaceList 'listName'
    Link ShellList 'listName'
    // 2.) Specify PressureHistory List(Req.)
    LoadCurveList 'PressureHistories'
  }
}
```

8.2.2 Uniform Pressure - Constant Face Areas

This list makes it possible to apply uniform pressure histories on a set of faces. In this case, the nodal forces are computed by multiplying the applied pressure to the initial surface area using the initial surface normal. This approach works well for LDPM models which experience major fragmentation. In some cases, some of the surfaces grow very large because fragments centered at the nodes move away from each other.

```
WetTriangFaceList 'ListName' {
  UniformPressureConstantFaces {
    // 1.) Specify face list (Req.), either a face list
    //     or a shell list
    FaceList 'listName'
    ShellList 'listName'
    // 2.) Specify either LoadCurve or Equation (Req.)
    LoadCurve 'curveName'
    Equation 'equationName'
  }
}
```

8.2.3 Multiple Pressure Histories

This list is used when pressure histories are independently computed by a CFD solver at certain stations on the exposed surfaces. The pressure histories are read into a LoadCurveList which is referenced here. This list uses the triangular faces of another list, either a face-list or a shell list. The faces in the parent list can change node definition, as it happens during fragmentation. However, if the parent list represents the external surfaces of a solid mesh and the number of faces increases as a result of solid fragmentation, this list will only employ the initial faces.

```
TriangFaceList 'ListName' MultiplePressureHistories {
    // 1.) Specify face list (Req.), either a face list
    //     or a shell list
```

```
    Link FaceList 'listName'
    Link ShellList 'listName'
    // 2.) Specify PressureHistory List(Req.)
    LoadCurveList 'PressureHistories'
    // 3.) Optional
    AutomaticTimeOffset // [1]
    TimeShift  345 ms   // [2]
  }
}
```

[1] The `AutomaticTimeOffset` command is designed to offset the time histories so that the pressure loads start at time 0. This is done by computing the first time pressures are different than 0. in any of the curves. All pressure histories are moved forward in time by that amount.
[2] The `TimeShift` command moves all pressure histories in time by the specified amount.
Time histories variables variables

8.3 Triangular DKT Shell List

This lists consists of flat triangular shell finite elements based on the discrete Kirchhoff (DKT) plate element formulation.

The input for this list include all the commands for the geometric triangular list, including generation, selection, and make commands. In addition, the following commands are available:

```
TriangFaceList 'ListName' DktShell {
  // commands from geometric shell list
  . . .
  // select one of the cross sections (required)
  SteelShell { m MATE i 3 }
  // specify a reference system for orienting local IP (optional)
  ReferenceSystem 'refSysName'
  // it is possible to run DKT with 2 or 3 IPs but 4 is better
  NumberGaussianPoints 4 // optional
}
```

If the reference system is not entered, then the global reference system is used. If the number of gaussian points is not entered, then the four integration points are used.

The specification of the reference system can be useful for specific geometries. For example, in the case of a cylindrical shell it is desirable to compute stresses in a cylindrical coordinate system, so that it would be easy to generate contour plots of the hoop or axial stresses. This is accomplished using the commands below

```
ReferenceSystem CylRS cylindrical {
  AxialDirection 0. 0. 1
  RadialDirection 1. 0. 0
```

```
}
TriangFaceList 'ListName' DktShell {
  . . .
  ReferenceSystem CylRS
  . . .
}
```

8.3.1 Time Histories

It is possible to save the histories of state variables for the DKT element. Note that there is a matrix of integration points: there are typically four sets of integration points over the surface of the element. Each set consists of the integration points through the thickness. Various combinations are possible and listed below.

```
TimeHistoryList 'listName' {
  . . .
  tfL-'shellList' 44  sv 1
  tfL-'shellList' 44  SIP 2 sv 1
  tfL-'shellList' 44  TIP 1 sv 1
  tfL-'shellList' 44  SIP 2 TIP 1 sv 1
}
```

If no surface point or thickness point is specified, then the average across of all points is takes. If a surface point is specified (`SIP 2`) then the average through the thickness is computed. If a thickness point is specified (`TIP`) then the average over the four surface point is computed.

9 Quadrilateral Faces and Shell Elements

9.1 Quadrilateral Face List

A quadrilateral face/shell list consists of a collection of homogenous two-dimensional 4-node elements. Currently, four types of sublists are available:

```
QuadFaceList 'listName' 'listType' {
  // list attributes
  FrontFaceColor gray // default  lightgray
  BackFaceColor red // default  lightgray
  // if this list is internally generated, enter
  Generate {
      . . .
  }
  // else if this list is derived from another list, enter
  SplitTriangFaceList TFLS
  // else if this list is specified via input, enter
```

```
  NodeList NODS // or
  InsertNodeList { . . . }
  ReadObjects 345
  //  i   n1   n2   n3   n4
      1  124  243   56  165
      2   56  238  121   78
      . . .
  // selection commands [optional]
  Select, Unselect, ... // see below
  Refine 2by2split // refine current mesh into 2x2 tiles
  Make EdgeList ListName AllEdges
  Make EdgeList ListName SharpEdges
  Make EdgeList ListName UnmatchedEdges
  // make FaceList of selected faces
  Make QuadFaceList ListName
  // make NodeList of nodes attached to selected faces
  Make NodeList ListName
  Write PartMeshDataFile ListName
  // use this command to read nodes and elements previously saved
  ReadFile PART.mrs
  SelectNodes   // [1]
  ReselectNodes // [1]
  UnselectNodes // [1]
}
```

[1] The `SelectNodes, ReselectNodes` and `UnselectNodes` commands are used to perform selection tasks on the nodes used in the definition of previously selected faces [or all faces]. The node selection can then be used in the node list for various other tasks.

9.1.1 Select commands

The selection commands are used to select a subset of the elements in the list.

```
Select [criteron]
AlsoSelect [criteron]
Unselect [criteron]
Reselect [criteron]
InvertSelection
[criterion] can take one of the following forms
all    // all faces
for 25  // face 25
for 1 5 // faces 1 through 5
for 1 100 2 // faces 1 through 100 step 2
1n // faces that have at least 1 node selected
4n // faces that have all 4 nodes selected
```

```
tw 0. 5. 4. // faces that point toward (0,5,4)
cp 1. 0. 0. > 0.5 // faces such that cross-product with 1,0,0 is greater than 0.5
```

Four-node face lists and all derived lists include commands for selecting nodes: `SelectNodes`, `UnselectNodes`, and `ReselectNodes`. See examples in the NodeList section.

9.1.2 Generate commands

The `Generate` sub-block is used for generating simple meshes of common geometries from within Mars. Multiple geometies can be generated and combined within the same block. The syntax for an input block is shown below. The specific inputs for each part are discussed in the next sections.

```
Generate {
  // enter one or more geometry feature
  Cylinder { . . . }
  Disk { . . .}
  Single { . . . }
  MergeParts // merge overlapping nodes [1]
}
```

[1] The `MergePars` command makes it possible to *fuse* two or more parts at the common nodes. This can be useful when generating more complex meshes, such as the mesh of a hollow cylindrical can with caps at both sides. Attention must be paid that the nodes on the edges overlap.

Cylinder

These commands generate a hollow cylinder

```
Cylinder {
  ReferenceSystem 'refSysName' // [1]
  EdgesOnCircle 36 // [2]
  Radius 4. in
  Length 10. in
  ElementSize 1. in  // in axial direction [3]
}
```

[1] This command employs a reference system which was previosly defined outside of the `QuadFaceList` section. The axis of the cylinder is aligned with the local z direction and spans from `z = 0` to `z = Length`. If the reference system is not specified, then the mesh is generated in the general reference system.

[2] No restrictions are given on the number of elements along the circumference.

[3] The size of the elements in the axial direction will be equal or less than the value entered.

Disk

```
Disk {
   ReferenceSystem 'refSysName' // [1]
   EdgesOnCircle 64 // must be multiple of 8
   Radius 4. in
}
```

[1] Same conventions as those ised for the `Cylinder`. The disk lays in the x-y plane and is centered at the origin.

Rectangular surface

```
Rectangle {
  LengthUnits in
  1 10 ; 1 6 ; // subd in x- and y- directions
  -5. 5.       // coord in x- and y- directions
  -5. 5.       //
  [ R PLAN ]   // in the x-y plane with corner at the origin
  0.           //
}
```

Triangular-based unstructured mesh

This generation method is suitable for generating a large class of coplanar unstructured meshes. The user must specify the outline of the surface. Any number of internal holes are also possible. Mars uses the program Triangle (see Plug-in section) which generates a triangular mesh. The output of Triangle is read back into Mars, which then splits each triangle into three quadrilateral faces. The mesh is generated in the X-Y plane. If a reference system is specified, then the mesh is rotated to that reference system. Note that the mesh can also be translated and rotated using the conventional commnads for node lists.

```
Triang-based {
  u in   // length units for this part
  R RSYS  // reference system [optional]
  L 0.15  // typical length of an element
  i  // invert quad orientation if necessary
  P // define polygonal external outline
  n 0.0 0.0  // first node of polygon
  n 1.0 0.0  // second node of polygon
  . . .
  c  // close the polygon
  //  enter internal circular holes (x, y, R)
  s 5  // min no. of sides in holes [optional]
  C 0.5 0.5 0.2 // [3]
```

```
  . . .
}
```

[3] Enter one line for each hole. The format is `C xc yc rad`, where `cx` and `yc` are the coordinates of the center, and `rad` is the radius. The hole should be fully contained inside the master polygonal surface.

Sphere

```
Sphere {  // free order
  R CYLN    // reference system
  r 4. in   // radius
  n 3       // n x 8 = number of circumferential elements
}
```

Duplicate

```
Duplicate {
  r 1 55 // range
  x 10 // time
}
```

Single Element

```
Single  4 in 6 in
// single element 4 in by 6 in laying in the x-y plane and centered at origin
```

Ring

```
Ring {
  R 'RefSysName'  // reference system
  // ring lays in local x-y plane
  // Specify either nce system
  D 4. in  // ring diameter
  d 2. in  // cross section diameter
  N 3      // number of subs around the ring
  n 3      // number of subs around the section
}
```

9.1.3 Make commands

The `Make QuadFaceList` is used for generating a sub-list of quadrilateral faces which have been previously selected. The new list is of the `Geometric` type; in other word, MARS will not perform any operation on it (e.g. computer internal forces).

The `Make EdgeList` command is used to generate a list of edges from the edges of the quadrilateral faces. This command must be terminated by a keyword for the edge selection criterion; three options are available:

```
  Make EdgeList 'listName' AllEdges
  Make EdgeList 'listName' SharpEdges
  Make EdgeList 'listName' UnmatchedEdges
```

The option 'AllEdges' is used to generate a list of all edges of the quadrilateral mesh. The option 'SharpEdges' is used to generate a list of edges for which the attached faces form an angle greater than 60 degrees. The option 'UnmatchedEdges' is used to generate a list of edges which are shared by a single face; note that if the surface is closed (e.g. a hollow prism), all edges are 'matched' and the generated edge list will be empty. The list generated using the 'SharpEdges' command includes unmatched edges.

9.2 Pressurized Quad Face List

These lists are used for applying pressure loadings on a set of quadrilateral faces. Several loading types are available:

1. Uniform pressure loading
2. Variable pressure loading
3. Special loads
4. Patched pressure histories

The general syntax for these lists uses the format below. More details are given for each specific loading tpye.

```
QuadFaceList 'listName' 'loadingType' {
  . . .
}
```

9.2.1 Uniform Pressure

This list is used for prescribing a time-dependent uniform pressure history over a set of quadrilateral faces. The pressure can be prescribed either using a 'LoadCurve' tabulated expression or using an 'Equation'. The latter is particularly useful when the pressures depend on the change in volume affected by the motion of the faces themselves. The single value time-dependent pressure is multiplied by the current area of each face in the direction opposite to its normal.

```
TrngFaceList 'ListName' UniformPressure {
    // 1.) Specify face list (Req.), either a face list
    //     or a shell list
    Link FaceList 'listName'
    Link ShellList 'listName'
    // 2.) Specify either LoadCurve or Equation (Req.)
    LoadCurve 'curveName'
    Equation 'equationName'
  }
}
```

9.2.2 Special Loads

This type of wet face list is used for situations when pressures can be defined as a function of time and initial face location. :

```
SpecialLoad 'Burst' ConWep {
  . . .
}
QuadFaceList 'ListName' SpecialLoad {
    // 1.) Specify face list (Req.), either a face list
    //     or a shell list
    Link FaceList 'listName'
    Link ShellList 'listName'
    // 2.) Specify SpecialLoad (Req.)
    SpecialLoad 'loadName'
  }
}
```

9.2.3 Multiple Pressure Histories

This list is used when pressure histories are independently computed by a CFD solver at certain stations on the exposed surfaces. The pressure histories are read into a LoadCurveList which is referenced here. This list uses the quad faces of another list, either a face-list or a shell list. The faces in the parent list can change node definition, as it happens during fragmentation. However, if the parent list represents the external surfaces of a solid mesh and the number of faces increases as a result of solid fragmentation, this list will only employ the initial faces.

```
LoadCurveList 'PressureHistories' {
  . . .
}
QuadFaceList 'ListName' MultiplePressureHistories {
    // 1.) Specify face list (Req.), either a face list
    //     or a shell list
    FaceList 'listName'
    ShellList 'listName'
    // 2.) Specify PressureHistory List (Req.)
    LoadCurveList 'PressureHistories'
    // 3.) Optional
    AutomaticTimeOffset // [1]
    TimeShift  345 ms   // [2]
  }
}
```

[1] The `AutomaticTimeOffset` command is designed to offset the time histories so that the pressure loads start at time 0. This is done by computing the first time pressures are

different than 0. in any of the curves. All pressure histories are moved forward in time by that amount.

[2] The `TimeShift` command moves all pressure histories in time by the specified amount.

9.3 Quad Shell Lists

```
QuadShellList NAME {
  // if this list is used to define a rigid body, enter
  Density 7.8 g/cm3
  // else select one of the cross sections
  SteelShell { m MATE i 3 }
  // reference system for local element axis alignment
  ReferenceSystem Local
  // default: 1st direction = diagonal nodes 1-3
  // select one of the formulation below
  QPH  // default
  Tsay // Belytshcko-Tsay formulation
  // if this list is not generated internally, enter
  NodeList NODS
  ReadObjects 345
  //  i   n1   n2   n3   n4   n5   n6   n7   n8
      1  124  243   56  165  234  312   23  126
      2   56  238  121   78   56   98  126   66
      . . .
#-- else
  generate {
#-- see below for generation options
  }
#-- optional commands
  Make tfL XFAC // generate a list of external surfaces
#-- select commands
  Select, Unselect, ... // see below
  Select, Unselect, ... // see below
  // Face Orientation commands
  OrientFaces Toward 0. in 0. in 7. in
  OrientFaces AwayFrom 0. in 0. in 7. in
  OrientFaces Direction 0. 1. 0
  EditNodeList {
    // nodlist commands
  }
  Write PartMeshDataFile PRT1.mrs
  Read PRT1.mrs
}
```

9.3.1 Weibull distribution

The Weibull distribution has been used very effectivley for characterizing probabilistic failure in materials and mechanical components. The probability density function is defined as

$$P(x) = \frac{g}{a}\left(\frac{x-m}{a}\right)^{(g-1)} \exp\left(-\left(\frac{x-m}{a}\right)^{g}\right) \quad \text{for} \quad x > m, \qquad = 0 \quad \text{otherwise}$$

where where

```
m: location parameter mu
a: scale parameter alpha
g: shape parameter gamma
```

The cumulative distribution function is defined as

$$F(x) = 1 - \exp\left(-\left(\frac{x-m}{a}\right)^{g}\right)$$

The input command is given by

```
Weibull { m 0.4 a 1. g 2 [ n ] }
```

where the optional 'n' is used to normalize the distribution.

9.3.2 Plot commands

```
QuadShellList PLAT {
  . . .
  PlotAttributes {
    ThickShells
  }
}
//-- To specify attributes in a PlotList file
PlotList PLOT {
  . . .
  qsL SHL1 { thk }   // thick plates
  qsL SHL2 {
    ThinShells
    vel RangeMaxValue 1000 in/s
  }
  qsL SHL3 { thn vel vmn 0. in/s  vmx 1000 in/s }
}
```

10 Tetrahedral Solid List

The `TetSolidList` includes a series of lists which implement collections of tetrahedral shaped elements. Some of the types of tetrahedral elements which are currently available is listed below:

- basic 4-node tetrahedral shapes,
- Lattice Discrete Particle Model (LDPM),
- viscous element used to artificially dampen internal motion,
- rigid disconnected elements,
- 4-node elasto-plastic element formulation,
- Cosserat formulation with 6 DoF's per node,
- explosive element which employs EoS for blast calculations,
- quadratic 10-node tetrahedral shapes and finite element formulations.

All these type are discussed in this section except for the LDPM elements which are discussed in a separate section, because of the great role that this method plays in Mars. The input format for tetrahedral list is given below:

```
TetSolidList 'ListName' 'type' {
  // where the keyword 'type' can be one of the following:
  // Geometry: this can be used to define rigid bodies
  // Explosive: this employs EOS materials
  // Ldpm: lattice discrete particle model formulation
  // Viscous: used to artificially dampen internal motion
  // if this list is used to define a rigid body, enter
  // 1. Material properties
  Density 7.8 g/cm3
  // else
  Material MATE
  // You can also use
  InsertMaterial Mat {
    . . .
  }
  // if material was not previously defined
  // 2. Specify mesh
  // if mesh is explicitly defined enter
  NodeList Nodes
  // or
  InsertNodeList Nodes {
    . . .
```

```
  }
  // if node was not previously defined
  // then, enter element definition
  ReadObjects 345 // number of elements
  //  i   n1   n2   n3   n4
      1  124  243   56  165
      2   56  238  121   78
      . . .
  // if mesh is internally generated, enter
  Generate {
    . . . // see below for generation options
  }
  // This command is also available
  MergeAllTetLists // {1}
  // 3. Modify mesh [optional commands]
  ImproveMesh  // remesh locally to eliminate slivers
  FlipMesh  'D' // D = 'X', 'Y', or 'Z' flip mesh
  // to make changes on the node list
  EditNodeList {
    . . . // nodlist commands
  }
  MergeNodes 'tol' // 'tol' is a dimensioned length
  // 4. Create additional lists [optional]
  Make TriangFaceList 'ListName' // generate external faces
  Make TetSolideList 'ListName' // generate list of selected tets
  Make EdgeList 'ListName' SharpEdgeds // generate edge list
  // 5. select commands
  Select, Unselect, ... // see below
  // use this command to save the mesh in a separate file
  Write PartMeshDataFile PART.mrs
  // use this command to read nodes and elements previously saved
  Read PART.mrs
  // use this command to write a table where
  // for each node we list its connectivity to
  // other nodes, number of tets, etc.
  Write ConnectivityData 'FileName'
}
```

1 This command is used to combine meshes from all previously defined tet solid lists. Currently, the original nodes from the parents lists are referenced in a new node list; the elements from the previous list are also referenced in the new list. For this reason, this command should be used in an intermediate mesh manipulation input file. The combined mesh should be written to an input file that can be later used in a more complex model.

10.1 Examples

```
TetSolidList RigidRing Geometry {
  Density 7.8 g/cm3
  NodeList RigidRingNodes
  ReadObjects 455
  . . .
}
TetSolidList Slab Ldpm {
  Material Concrete
  Read Slab.mrs
}
```

10.2 Select Commands

These commands are used to select a subset of elements on which to operate

```
  Select [criterion]
  AlsoSelect [criterion]
  Unselect [criterion]
  Reselect [criterion]
  InvertSelection
  [criterion] can take one of the following forms:
    all    // all elements
    do 25  // element 25
    do 1 5 // elements 1 through 5
    do 1 100 2 // elements 1 through 100 step 2
    vl > 0.4 // elements with volume > 0.4
    vl = 0.4 // elements with volume apprx = 0.4
    vl < 0.4 // elements with volume < 0.4
    1n // elements with at least one node selected
    4n // elements with all four nodes selected
Examples:
  Select do 1 100 // select element 1 through 100
  AlsoSelect do 201 300 // add elements 201 - 300
  Reselect 4n // select only element with all four nodes
              // selected from elements selected above
```

Tet solid lists and all derived lists include commands for selecting nodes: 'SelectNodes', 'UnselectNodes', and 'ReselectNodes'. See examples in the NodeList section.

10.3 Generate Commands

The `Generate` command is used for generating tetrahedral meshes of simple geometries. Within the `Generate` subsection a single or multiple parts can be generated. If multiple parts are generated some nodes of these parts share the same locations, these nodes

can be merged using the t[mergeParts] command. The general format of the `Generate` subsection is shown below:

```
TetSolidList NAME {
  Generate {
    // generate one or more parts using commands discussed below
     . . .
    // merge parts when distance between nodes is < tol
    mergeParts 0.001 in // tol = 0.001 in
  }
}
```

Cylinder

The `Cylinder` command is used for generating a regular tetrahedral mesh of a solid cylinder or of a section of a pipe.

The following example generates a hollow cylinder with internal diamter of 2. in and external diameter 2.31 in. The cylinder extends in the z- direction from z = 0.3 in to z = 19.52 in with 9 elements

```
    Cylinder { // use ingrid convention
      5 6 ; 1 10 ;
      2. 2.31   // radii
      0.3 19.52 // coordinates in the axial (z) direction
    }
```

Prism

The `Prism` command is used for generating a structured tetrahedral mesh of a parallelepipedal shape.

```
/* Generate a prism with regular grid
    Parallelepiped { // use ingrid convention
      1 5 ; 1 3 ; 1 3 ;
      -4. 4.
      -2. 2.
      -2. 2.
    }
```

Extrusion

The `Extrusion` command is used for generating an extruded solid starting from a triangular mesh defined in the x-y plane. The triangular mesh is extruded in the z-direction starting from z = 0 and ending at z = `Length` with element dimension in the z direction no larger than `Increment`.

```
Extrusion {
  TriangularFaceList 'listName'
  Length 10 in
  Increment 1 in
}
```

Solid Disk

```
Disk { // use ingrid convention
  0 6 7 ; 0 1 2 ;
  0. 2. 2.31
  0. 0.3 0.6
  d 6 7 ; 0 ;
  d 5 7 ; 1 ;
  d 0 2 ; 2 ;
}
```

10.4 Make Commands

The `Make TetSolidList` is used for generating a sub-list of all tet elements which have been previosly selected. The new list is of the 'Geometric' type; in other word, MARS will not try to compute internal forces.

The `Make TriangFaceList` is used for generating a list of all triangular external faces of the complete mesh. If the user desires to generate external faces of a portion of the mesh, then the 'Make TetSolidList' command should be done first and the face list should be generated from inside the tet sub-list.

The `Make EdgeList` command is used to generate a list of edges from the edges of the tetrahedral elements. This command must be terminated by a keyword for the edge selection criterion; three options are available:

```
Make EdgeList 'ListName' AllEdges
Make EdgeList 'ListName' SurfaceEdges
Make EdgeList 'ListName' SharpEdges
```

The option `AllEdges` is used to generate a list of all internal and external edges of the tet mesh. The other two options rely on the list of external tet faces generated using the 'Make TriangFaceList' command. If the triang-face list was not generated, MARS will automatically generate it. The option `SurfaceEdges` is used to generate all external edges of the tet mesh. This list is useful for edge-edge contacts. The option `[SharpEdges` is used for generating a list of edges for which the attached faces form an angle greater than 60 degrees. This list is useful for graphics when we want to represent the outline of a solid component.

10.5 Time History Commands

The following line commands are intended to be used inside Time History lists to produce records of global and element variables.

```
TimeHistoryList HIST {
  . . .
  // histories for entire list
  ttL-PART Volume
  ttL-PART InternalWork
  ttL-PART DissipatedEnergy
  // histories for single element
  tt-PART 1 Volume // element 1 only
  tt-PART 1 StateVariable 3
}
```

For internal work we intend the work done by element internal forces which results in recoverable elastic energy and dissipated energy

10.6 Plot Attribute Commands

Plotting attributes can be specified in the element list or in the plot list

```
TetSolidList PART {
  . . .
  PlotAttributes {
    ContourVariable sv 1
    NoNodalAveraging
    NoSmoothing
  }
}
PlotList PLOT {
  . . .
  ttL PRT1 {
    ContourVariable sv 1
    NoNodalAveraging
    SelectedElementsOnly
    NoSmoothing
  }
  ttL PRT2 { OutlineOnly }
}
```

10.7 Viscous Tets

The purpose of this list is to provide some form of artificial internal damping to kill internal vibrations. It is different than dynamic relaxation in the fact that a vibrating

moving body will stop vibrating but its average velocity is maintained. This list is used in conjunction with another list consisting of deformable elements. This list does not own its objects (tets), but uses the objects of the tet list it is connected to.

```
TetSolidList 'ListName' Viscous {
  // 1.) Enter master list (Req.)
  MasterTetList 'TetListName'
  // 2.) Enter either load curve or damping constant (Req.)
  LoadCurve 'CurveName'
  Damping  0.001 1/s
}
```

Prescribing the damping coefficient as a function of time using the `LoadCurve` option makes it possible to use this feature for computing steady state static solutions. Damping can then be removed when applying dynamic loads.

The viscous force between nodes J and K in direction i is computed using the equation

$$f_{iJK} = C\ (m_J + m_K)\ (v_{Ji} - v_{Ki}) \qquad i = x,\ y,\ z$$

where C is the damping coefficient.

10.8 Spatial Field Functions

The purpose of this list is to provide a spatial field of a scalar variable that affects material properties at the integration points of finite elements or Ldpm elements. Such variable could be temperature, irradiation, water level, etc. Typically, these fields would be computed by another special purpose code. For this list, the spatial distribution of a variable f is specified at the nodes of a tetrahedral mesh. If the field is constant during the simulation, then a single record is sufficient. If the field varies in time, then a series of records is specified at different times. This list is used in other lists. For example, let's assume that the mechanical properties of a material are temperature dependent and we have computed the temperature history and distribution. Then, the code would interpolate the temperature at the integration points, both in time and space. The scalar field mesh and the finite element mesh do not need to be the same. However, the scalar field mesh should contain all integration points of the finite element mesh. The input commands for this list are:

```
TetSolidList 'listname' ScalarField {
   // define tet solid mesh using standard commands such as:
   InsertNodeList { }
   ReadObjects 'no.tets'
   . . .
   // enter list specific commands
   NumberOfStates 'n' // [1]
   TimeUnits h // [2]
```

```
   ReadDataFile 'filename'
   PlotDataSet [3]
}
```

This list must be entered before it is used in other lists. In the example below, we define a history for the humidity distribution in a volume of concrete in list `Humidity` . In the LDPM list, the scalar field HumidityField is assigned to the state variable labeled Humidity. Humidity.

```
TetSolidList HumidityField ScalarField {
  . . .
}
TetSolidList 'listname' Ldpm {
  . . .
  ScalarField TetList HumidityField StateVariable "Humidity"
  . . .
}
```

The data file is an ASCII file with the following structure:

```
t(0)
f(0,1) f(0,2) f(0,3) ...  f(0,nnd)
t(1)
f(1,1) f(1,2) f(1,3) ...  f(1,nnd)
 . . .
t(n)
f(n,1) f(n,2) f(n,3) ...  f(n,nnd)
```

The function scalars f(t,i) must be separated by at least a space and can be written in multiple lines. nnd is the number of nodes in the mesh:

[1] The number of states is used to read the first 'n' datasets in the datafile. If 'NumberOfStates' is missing or 'n' is greater than the number of states in the datafile, the program will stop when the eof is reached.

[2] If the 'TimeUnits' commands is missing, MARS assumes that times are given in the default time units, which is typically seconds.

[3] The optional 'PlotDataSet' command is used for generating a sequence of Quasar contour plots for the field variable. The name of the files is the same as the name used for the list. For example, if the list name is 'Temperatures', the sequence of plot files will be 'Temperatures.000', 'Temperatures.001', etc.

10.9 Ten-Node Tet Elements

The ten-node tet element is essentially a four-node tetrahedral element with six additional nodes placed along the six edges of the element. Typically, the six nodes are placed at the midpoint of the edge. However, if the edges are located on a curved external surface of a

part, the midpoint edges should be placed on the curved surface for improved geometric definition.

The are two ways for defining a ten-node tet mesh: 1. define a four-node tet mesh and then insert the mid-edge nodes, 2. generate a ten-node mesh using a commercial mesh generation package and read the mesh directly into Mars. The first method employs the following input format:

```
TetSolidList 'listname' 10NodeElement {
   // Define 4-node tet mesh using standard commands
  InsertMidEdgeNodes
   . . .
}
```

The second method employs this input format:

```
TetSolidList 'listname' 10NodeElement {
  InsertNodeList {
    . . .
  }
  ReadObjects 45
  1  n1-1 n1-2 n1-3 . . . n1-10 // [1]
  2  n2-1 n2-2 n2-3 . . . n2-10
  . . .
}
```

[1] The indexing system follows these rules:

- node 5 between nodes 1 and 2
- node 6 between nodes 2 and 3
- node 7 between nodes 3 and 1
- node 8 between nodes 1 and 4
- node 9 between nodes 2 and 4
- node 10 between nodes 3 and 4

Note that the `10NodeElement` keyword in the first line is used for defining a purely geometric mesh with no elasto-plastic properties. Ten-node finite element formulations are listed below.

10.9.1 Ten-Node Small Deformation Element

The 10-node small deformation tet element formulation is intended to be used for cases where the deformations are small. A good description of the 10 node tet formulation is given in www.colorado.edu/engineering/CAS/courses.d/.../AFEM.Ch17.pdf. A nice property of the T10 element is that it is not overconstrained nor underconstrained: it features 10 nodes x 3 DOF/node = 30 DOFs in total, 4 integration points each providing 4 IP x 6 constrant/IP = 24 constraints, which leaves 6 unconstrained DOF's: the six rigid body motions. The formulation for small deformations save computing time by assembling the B-matrix only once at the beginning of the simulation, and by not rotating the stress tensors at the integration points during the simulations, since rotations are assumed to be small.

This formulation is invoked using the following commands:

```
TetSolidList 'listname' 10NodeSmallDef {
  Material 'materialName'
   . . .
```

10.9.2 Ten-Node Large Deformation Element

The 10-node large deformation tet element formulation is similar to the small deformation formulation with two significant differences: 1. the B matrix is computed at every step, and 2. the stress tensor is rotated to account for large rotations. The latter is accomplished by attaching a local reference system (LRS) to each of the four integration points. The orientation of the LRS is updated using the spin tensor. Strain rates computed in the global reference system (GRS) are rotated to the LRS and used to update the stress tensor. Note that the stress tensor is always defined in the local reference system. The local stress tensor is then roated to the GRS and used to compute the nodal forces.

This formulation is invoked using the following commands:

```
TetSolidList 'listname' 10NodeLargeDef {
  Material 'materialName'
   . . .
```

11 Lattice Discrete Particle Model

The Lattice Discrete Particle Model (LDPM), is a discrete meso-mechanical model for concrete, which was recently developed by Dr. Cusatis and co-workers at Rensselaer in collaboration with Dr. Pelessone at ES3. LDPM simulates the mesostructure of concrete by a three-dimensional assemblage of discrete particles whose position within the volume of interest is generated randomly according to the given aggregate size distribution. A three-dimensional domain tessellation, based on the Delaunay tetrahedralization of the generated aggregate centers, generates a system of cells embedding the aggregate particles and interacting through triangular facets. A mesoscale constitutive law governs

the interaction between adjacent cells and it simulates various features of the mesocale response, including cohesive fracturing, strain softening in tension, strain hardening in compression, material compaction due to pose collapse, frictional slip, rate and creep effect for dynamics, etc.

LDPM has been extensively calibrated and validated in the last few years and it has shown superior capabilities in reproducing and predicting qualitative and quantitative concrete behavior under a wide range of loading conditions.

LDPM was also used successfully to the simulation of projectile penetration, blast, and fragmentation. Figs. 2a-g (Figures will be included in later version of the manual) show a gallery of some of the results obtained using LDPM. Fig. 2a shows LDPM simulation result for mixed mode fracture. The simulation is relevant to a four point bending test of a specimen with two notches. As observed in experiments, two curved fractures propagate from the notch tips towards the opposite sides of the specimens. In Fig. 2b a snapshot of a blast simulation is shown. Fig. 2c is depicts the impact of a steel rod onto a concrete block. As observed in reality the number of fragments increases with the initial impact velocity and there is a transition from a failure with localized cracks (left) to a failure with complete fragmentation (right). Fig. 2d shows the formation of shear bands at failure for a specimen subjected to uniaxial compression. Fig. 2e presents the LDPM model, damage distribution, and crater formation for a simulation of projectile penetration through a reinforced concrete slab. The LDPM framework can also handle coupling with steel reinforcement. The concrete-rebar bond model is obtained through a penalty formulation that allows the simulation of nonlinear bond slipping. Fig. 2f shows the simulation of a dynamic pull-out test leading to splitting failure. Finally, Fig. 2g shows the LDPM capability of handling complex three-dimensional fracture paths with multiple branching and crack coalescence.

Recently, LDPM was extended to include the effect of fiber reinforcing. The updated formulation, named LDPM-F, incorporates the effect of fibers by modeling individual fibers, placed within the LDPM framework according to a given fiber volume fraction. The number and orientation of fibers crossing each facet is computed, and the contribution of each fiber to the facet response is formulated on the basis of a previously established micromechanical model for fiber-matrix interaction

Currently, LDPM-F is being applied to the simulation of the CORTUF concrete developed by ERDC. Preliminary results clearly demonstrate the ability of LDPM to model the micromechanical phenomena characterizing CORTUF failure

11.1 Input commands

```
TetSolidList 'listname' LDPM {
  // define tet solid mesh using standard commands such as:
  InsertNodeList { }
  ReadObjects 'no.tets'
  . . .
  // enter list specific commands
  DisableFiberFacets { // [1]
    FiberRadius 0.02 in
```

```
    // enter either an EdgeList or BeamList
    EdgeList 'FiberListName'
  }
  WriteStateVariableDumpEvery 0.010 ms // [2]
  WriteCellDataDump 'fileName' // [3]
  WriteFacetDataDump 'fileName' // [4]
  ScalarField TetList 'listname' StateVariable 17 // [5]
  ScalarField TetList 'listname' StateVariable "Temperature"
  ScalarField HexList 'listname' StateVariable 18
  FacetScalarField {    //  [6]
    InputFile 'filename'
    StateVariable 'VariableName'
  MassScaling // [7]
}
```

[1] The `DisableFiberFacets` command is used in conjunction with t[ParticleFiberInteractionList] to disable LDPM facets, whose centers are located inside the fibers. The algorith computes the minimum distance of each facet from all edges in the edge or beam list. If the distance is less than the fiber radius parameter, then that facet is disabled and no longer participates in the calculation. Following is an example of how to use it. Obviously, the beam lists in the t[TetSolidList] and `InteractionList` should be the same, while the fiber radius could be different.

```
BeamList Fibers { }
TetSolidList 'listname' LDPM {
  . . .
  DisableFiberFacets {
    FiberRadius 0.02 in
    BeamList Fibers
  }
}
ParticleFiberInteractionList BottomHalf {
  . . .
  BeamList Fibers
  FiberRadius 0.02 in
}
```

[2] The `WriteStateVariableDumpEvery` command is used for generating a family of ASCII files named `LdpmStVarDump.xxxxxx` at periodic time intervals. The `xxxxxx` string is actually the time in microseconds; for example, `LdpmStVarDump.001240` contains all facet state variables at time 1.240 ms. Each file is structured in blocks of 13 lines, one block for each Ldpm tet element. The first line contains the element index, the following 12 lines contain the state variables for the 12 facets.

[3] The `WriteCellDataDump` command is used for writing an ASCII output file containing all information necessary to characterize the geometry of all the Ldpm cells in

the model. This file is printed once at the beginning of the simulation. The structure of the output file is as follows

```
// For each cell
Cell jc         // index of particle at the center of the cell
//  Coordinates of the center particle/node
crd: cx cy cz
//  Total volume of cell
vol: V
//  Number of outside points defining cell
nxp: np
//  Local coordinates of outside points follow
x1 y1 z1
x2 y2 z2
. . .
//  Number of facets internal to the solid and shared with other cells
nif: nf
//  Facet connectivity and facet areas follow
j1t j1f  i1.1 i1.2 i1.3  A1  n1.x n1.y n1.z
pA1   p1.x p1.y p1.z  q1.x q1.y q1.z  s1.x s1.y s1.z
j2t j2f  i2.1 i2.2 i2.3  A2  n2.x n2.y n2.z
pA2   p2.x p2.y p2.z  q2.x q2.y q2.z  s2.x s2.y s2.z
. . .
where jkt is the index of the tet element that contains facet k,
      jkf is the facet index (1-12) of the facet withing the tet element,
      ik.1, ik2, ik.3 are the indeces of the outside points that define facet k,
      Ak is the actual area of facet k
      nk.x nk.y nk.z is the normal to facet k (not projected)
      pAk is the projected area
      pk.x pk.y pk.z is the normal to the projected face
      qk.x qk.y qk.z is the first tangential direction
      sk.x sk.y sk.z is the second tangential direction
//  Number of facets on the external solid surface sharing center node
nxf: nf
//  Facet connectivity and facet areas follow
//  Index 0 refers to center node
i1.1 i1.2 i1.3  A1
i2.1 i2.2 i2.3  A2
. . .
//  Total number of edges in the cell
nxe: ne
//  Edge connectivities and edge lengths follow
i1.1 i1.2  L1
i2.1 i2.2  L2
. . .
```

```
where ik.1, ik2 are the indeces of edge k,
      Lk is the length of edge k
```

[4] The `WriteFacetDataDump` command is used for writing an ASCII output file containing all information for the 12 facets of each tetrahedral LDPM element. The output data is structured as follows:

```
For each tet
  Tet 'index'
followed by 24 lines, two for each facet
  n1 n2  cx cy cz  fa  nx ny nz
  pa   px py pz  qx qy qz  sx sy sz
where:
  n1:  index of first node on facet edge
  n2:  index of second node on facet edge
  cx, cy, cz: coordinates of facet center
  fa: area of facet
  nx, ny, nz: normal to facet
  pa: projected area (used in calculations)
  px, py, pz: normal to projected facet
  qx, qy, qz: first tangential direction
  sx, sy, sz: second tangential direction
```

Note the node indeces n1 and n2 are also the cell indeces.

[5] The `ScalarField` command is used for specifying a time dependent spatial scalar field, such as temperature, humidity, etc. The scalar field is actually specified in a separate list, which must be entered prior to the definition of the current Ldpm list. For details on how to enter a scalar field list, see specific sections of the manual. The meshes for the scalar field and for the LDPM model can be different; indeed, one can use either a tetrahedral solid mesh or an hexahedral solid mesh. The scalar field is interpolated at the center point of the facets of the LDPM model. Furthermore, the values at the facets are interpolated in time. The interpolated scalar is assigned to the state variable specified in the command. The state variable can be identified either by its index or its description, as it appears in the material state variable table. Note that the material model must be designed to accomodate the specified state variable.

[6] The `FacetScalarField` command is used for specifying a time dependent scalar filed (see above) directly at the facets. The data is read from an input file that has the following format:

```
t1
f1-1-1 f1-1-2  ...  f1-1-12
f1-2-1 f1-2-2  ...  f1-2-12
 . . .
t2
f2-1-1 f2-1-2  ...  f2-1-12
```

```
f2-2-1 f2-2-2  ...  f2-2-12
 . . .
where
  ti: is the time for the i-th record
  fi-j-k: is the value of the scalar field for j-th element,
          k-th facet, i-th record.
```

The values of the scalar at the facets are interpolated in time. The interpolation time is the time when the forces are calculated. Up to 10 scalar fields can be specified.

[7] The `MassScaling` command is used to increase the mass of elements that have very small Courant time steps. Typically, in large meshes there are a few poorly shaped elements (slivers, flat elements, etc.) that would force the entire simulations to run using small integration time step. It is a common practise to increase the density of these elements, because their mass is very small anyway. The time steps for Ldpm elements is computed by assemblying the stiffness matrix and computing its maximum eigenvalue e. The time step dt is then defined as

$$dt = 2.\sqrt{\frac{1.}{e}}$$

These operations are performed during the initialization phase. A summary of these operations is printed to the output file and looks like this:

```
Min. time step for stability:   808.24e-9 s
510 tets were made heavier
Current min. time step :  1000.00e-9 s
Actual total mass    :    0.914831 kg
Adjusted total mass  :    0.924320 kg
Percent mass increase: 1.03727%
```

Note that the operations for computing the time steps are quite expensive but need to be done only once. Since Oct. 2011, the stable time steps for all elements are automatically computed and saved to a binary file named using the following convention `ttL-'listName'.cts`. The next time the same model is run, Mars looks for this file and reads the previously saved time steps. Since Oct. 2011, Mars performs further checks to ensure that the .cts file corresponds to the current model: first it checks that the number of elements is the same, then it computes the stable time step for the first element and compares it with the value in the file. If either test fails, Mars automatically deletes the .cts file and exits with an error message prompting the user to resubmit the job. If `MassScaling` is not used, the minimum time step for the Ldpm list is used in the computation of the global integration time step.

11.2 Model Generation

Because of the unique requirements of LDPM models, a series of special purpose of mesh generation methods are made available.

```
TetSolidList 'listName' LDPM {
  Material 'materialName'
  Generate {
    // choose one of the options
    LdpmBox { . . . }
    LdpmCylinder { . . . }
    LdpmSphere { . . . }
    . . .
  }
}
```

11.2.1 Box

The `LdpmBox` command is used for generating an LDPM concrete parallelepipedal box. This method first generates points along the edges of the box, then points on the faces of the box. It then randomly places a set of particles inside the box. It uses tetgen to generate a tetrahedral mesh. The method selects an appropriate mesh density for the exernal mesh based on expected average distance between internal particles.

```
LdpmBox {
  Dimensions 4 in 2 in 8 in   // dimension in x, y and z directions [1]
  [ Seed 23423 ]  // seed for random number generator
  [ ConstantSpacedParticlesOnEdges ]
}
```

[1] The box spans from 0 to 4 in in the x-direction, from 0 to 2 in in the y-direction, and from 0 to 8 inches in the z-direction.

11.2.2 Cylinder

The `LdpmCylinder` command is used for generating an LDPM concrete cylinder. This method first generates an external triangular face mesh representing the surface of the cylinder. It then randomly places a set of particles inside the cylinder. It uses tetgen to generate a tetrahedral mesh. The method select an appropriate mesh density for the exernal mesh based on expected average distance between internal particles.

```
LdpmCylinder {
  // automatically generates particle list PRTC
  Radius 2 in   // radius of the cylinder
  Diameter 4 in // use either Radius or Diameter
  Length 8 in   // length of the cylinder
  GapScalingFactor 0.1 // gap between particles
[ Seed 23423 ]  // seed for random number generator
}
```

11.2.3 Sphere

The `LdpmSphere` command is used for generating an LDPM concrete sphere. This method first generates an external triangular face mesh representing the surface of the sphere. It then randomly places a set of particles inside the sphere. It uses tetgen to generate a tetrahedral mesh.

```
LdpmSphere {
  // automatically generates particle list PRTC
  Radius 2 in   // radius of the sphere
  Diameter 4 in // use either Radius or Diameter
  Refinement 3  // [1] external mesh density
[ Split ] // generate only half sphere for mesh check
[ Seed 23423 ]  // seed for random number generator
}
```

[1] The argument of the `Refinement` parameter is an integer that represents the level of refinement of the external mesh. For a value of 1 (lowest resolution) the sphere is approximated with an octahedron. For each increment, each triangle is subdivided into four triangles making the mesh finer. The level of resolution should be consistent with the internal mesh. This can be visually checked using the `Split` command, which makes it possible to split the sphere in two parts across the middle and look at its interior

11.2.4 DogBone Specimen

```
DogBoneSpecimen {
  Material Concrete
  Seed 5405
  h 4 mm //  typical mesh length
  Long   //  for defining long specimen
  Plot   //  plot intermediate steps
}

DpVolume {
  // automatically generates particle list PRTC and
  // tet mesh given a triang. face defined volume
  tfL VOLM
[ Seed 23423 ]  // seed for random number generator
}
FromExternalFaceList listName
```

11.3 Time Histories

The LDPM elements employ the same time history commands as the regular tetrahedral element. The only additional feature is the ability to plot state variables at any of the twelve facets.

```
   tt-'listName' 'jt' Facet 'jf' StateVariable 'jsv'
```

where `jt` is the index of the Ldpm element, `jf` is the index of the facet (1 through 12), and `jsv` is the index of the state variable.

11.4 Using Pre-Generated Meshes

The typical way of performing LDPM simulations is to first generate a LDPM mesh of the specimen or component using one of the techniques described in the previous section and then to create a full model which employs the mesh generated earlier. In the generation phase, the mesh is saved using the `Write PartMeshDataFile` command. The data file has the following structure

```
  InsertMaterial CONC RCConcrete Dev { . . . }
  InsertNodeList PRTC { . . . }
  ReadObjects 'n'
  // element connectivity
EOF
```

Note that unlike other mesh datafiles, the LDPM datafile includes commands for defining the material object that was used to size and distribute the LDPM particles.

In older versions of Mars, it was possible to define a concrete material model before the `TetSolidList` is defined and use it in the `TetSolidList` in this fashion

```
Material Concrete RCConcrete Dev { . . . }
TetSolidList 'ListName' LDPM
  Material Concrete
  ReadFile specimen.mrs
  . . .
}
```

In this input scenario, the `InsertMaterial` command in file `specimen.mrs` would have replaced the externally defined material `Concrete` with the material saved in the datafile. The user would have been unaware of that. Since May 26, 2011, this is no longer possible. In the current version, an error trap has been placed and the material can only be defined once.

It is possible to change material parameters inside the `TetSolidList` using the `EditMaterial` command

It is possible to change material parameters inside the `TetSolidList` using the `EditMaterial` command

```
TetSolidList 'ListName' LDPM
  ReadFile specimen.mrs
  EditMaterial {
    // use standard input commands for RCConcrete model
  }
}
```

11.5 Stable Element Time Steps

Stable time steps for each LDPM element need to be computed to ensure that the time step used in the solver is small enough to avoid local (or global) instabilities during the simulation. The computation of the Courant stability time step for an LDPM requires the assembly of the element stiffness matrix (24x24 size) and the solution of its largest eigenvalue. As such, this is a computationally expensive operation. Unlike ductile steel materials, concrete material do not experience significant plastic deformations before fracturing. Thus, the geometry of LDPM elements remain fairly constant during simulations and there is no need to recompute stable time steps. The computation of the stable time steps is only done once at the beginning of the simulation.

Furthermore, logic has been placed so that stable time steps are saved in a file named `ttL-ListName.cts`. As of April 2012, when MARS initializes an LDPM list, it first looks for the `cts` file in the current folder. If it finds it, it will try to use the steps computed in a previous simulation. Two checks are performed to ensure that the data is usable: 1. the number of elements in the list must be the same as the number of time steps in the `cts` file, 2. the computed time steps for the first ten elements in the list must be the same as the values of the time steps in the `cts` file. The second check is intended to account for conditions when the elastic properties of the material are changed during the calibration process. If either condition is not satisfied, then the time steps for all elements are recomputed and saved to the `cts` file, possibly overwriting previous data. This activity is documented in the output file as shown in the example below.

```
Initializing list ttL-PRTC
  Element time steps read from file ttL-PRTC.cts
  Time steps in *.cts are not usable (properties may have changed)
  Stable element time steps are recomputed.
  Min. time step for stability:   316.32e-9 s
  Time steps saved in file ttL-PRTC.cts
```

Unlike previous versions of MARS, where the `cts` file had to be explicitely deleted by the user to eliminate errors during execution, the current version of MARS does all the operations automatically and the process is transparent to the user. It is still a good idea to periodically check the output and see what operations are performed.

11.6 LDPM Visualization

There are essentially two classes of methods for visualizing LDPM models: tet-based methods and cell-based methods. Tet-based methods were the first to be implemented. Cell-based methods require more memory for storing additional data but provide more realistic erenderingentations of the cracking process; their additional computational cost is insignificant. Tet-based methods are no longer discussed in this manual as they generate lower quality graphical representations. Cell-based methods and various applications are discussed below.

Cell plot rendering provides a more realistic representation of the fracturing process for two reasons: material does not disappear and cracks are clearly visible. The idea

behind this rendering is to plot visible faces from all cells of a model. Since it would be computationally very expensive to plot all internal facets; MARS checks the value of the crack opening and if it exceeds an input value, it assumes that a large enough crack has formed and both faces of the facets are plotted. All external facets are always plotted. Facets edges are also plotted when the internal facets are plotted. Figure 4 shows a fractured brick. The relevant input for this example is listed below. Currently, the parameter to control plotting of cracked surfaces is specified inside the TetSolidList and is defined by the keyword `CrackOpening`. A cell plot of an LDPM model can be requested inside a `PlotList` with the command `ttL Brick { Cells }`. Since July 2011, the definition of the crack opening parameter can be made inside the plot lists using the command `MinimumCrackOpening`. Notice that the level of detail in crack displaying can be controlled by varying the value of the crack opening parameter. Making that value too small may make the plot too busy.

Most plotting capabilities are available for both Quasar and Paraview. Quasar will not work reliably and efficiently for very large models, but it will display a final image very quickly (when it can) since it does not require a long set-up procedure. Paraview provides great capabilities for changing properties and attributes of graphical components and can process very large models. Unlike Quasar which combines components in a single files, Paraview requires graphical components to be specified in different families of files. As such, the way `PlotLists` are specified for the two codes is different. For example, if we want to generate a contour plot of external facets in solid color and contour plot of crack opening for the internal facets, the Quasar input would be set up using a single `PlotList`

```
PlotList CrackOpening {
  TimeInterval .01 ms
  ttL Tile { ExternalCellFacets }
  ttL Tile {
    FacetVariable 15
    MinimumCrackOpening 0.01 mm
    RangeMinValue 0.01 mm
    RangeMaxValue 0.1 mm
  }
}
```

while the input for for Paraview must be broken up into two separate `PlotLists`

```
PlotList TileExtFaces {
  Paraview
  TimeInterval .01 ms
  ttL Tile { ExternalCellFacets }
}
PlotList Contours {
  Paraview
  TimeInterval .01 ms
```

```
  ttL Tile {
    FacetVariable 15
    MinimumCrackOpening 0.01 mm
    RangeMinValue 0.01 mm
    RangeMaxValue 0.1 mm
  }
}
```

11.6.1 Plotting cell facets

The `Cells` plot option makes it possible to combine external and internal cell facets into a single triangular face list. As discussed earlier, the visibility of the internal facets is controlled by the `MinimumCrackOpening` parameter. Decreasing this parameter makes the number of internal facet larger slowing down their rendering.

```
PlotList 'Name' {
  . . .
  ttL 'ListName' {
    Cells
    MinimumCrackOpening 0.01 mm
  }
}
```

This plotting method is available for both Quasar and Paraview.

11.6.2 Plotting external facets only

A variation of `Cells` method makes it possible to plot only the cell triangular facets that are initially visible. Essentially, these are the external facets of the tet mesh which are not shared by two adjacent cells. The number of facets in this list does not change during the simulation. I can be used for quickly assessing the progress of a simulation or for coupling with with facet contour plots and displaying the external surface in a neutral color since they are not part of the contour facet list. The command for displaying external faces is is

```
  ttL 'ListName' { ExternalCellFacets }
```

This option is available for both Quasar and Paraview.

11.6.3 Plotting cell outline

If the option of displaying sharp edges is required, the command `CellOutline` creates a list of edges that are visible. The initial list would include the sharp edges of the initial mesh. As the Lpdm model breaks up, the edges of the cells that have separated from the bulk of the model, may be displyed depending on the angle of the facets sharing an edge. edge.

```
ttL 'ListName' { CellOutline }
```

The line lists generated using the `CellOutline` command can become very large and the plot may show too many edges. In these cases, it is preferable to display only the initial sharp edges of the model in their current location. This is accomplished by the command `CellInitialOutline`

```
ttL 'ListName' { CellInitialOutline }
```

11.6.4 Plotting particles

This feature provides the capability of plotting particles as spheres. It is no different than the plotting option available for standard `NodeLists`.

```
ttL 'ListName' { Particles }
```

This option is available for both Quasar and Paraview.

11.6.5 Plotting embedded fibers

If the component contains embedded fibers, these can be plotted using the command `Fibers`

```
ttL 'ListName' { Fibers }
```

This option is available for both Quasar and Paraview.

11.6.6 Contour plotting of facet variables

This plotting feature provides the ability to display state variable information at the facet level. As for the `Cells` plot, the total number of facets can be very large. For this reason, there are options for reducing the number of facets included in the facet list, which are eventually plotted. The variable to be plotted is selected using the `FacetVariable` keyword followed either by the variable index or the variable label. These can be chosen from the list of state variables for the material being used. The first level of filtering is obtained using the command `MinimumCrackOpening` which works in the same fashion as in the `Cells` plot. In addition, if a variable range is specified using either or both `RangeMinValue` and `RangeMaxValue`, then the facets for which the variable is outside the range are removed from the list.

```
ttL Block {
  FacetVariable 15 // crack opening variable
  MinimumCrackOpening 0.01 mm
  // do not use next four options for paraview plots
  RangeMinValue 0.01 mm
  RangeMaxValue 0.10 mm
  DisplayBelowMin
```

```
    DisplayAboveMax
    Scale 1000 // convert from m to mm
  }
```

The last three options should be omitted for Paraview plots, since the same functionality is obtained in Paraview in the ObjectInspector > Display > EditColorMap form and using the threshold filter.

11.6.7 Domain decomposition plots

The following example shows the commands for generating a Paraview file which contains the exploded view of a tet-list depicting the domain decomposition. The parameter 1.3 controls the amount of radial motion for the domains. The coordinates of the center of gravity of each domain are multiplied by this parameter. A value of 1. means the components stay where they are. The larger the value of this parameter, the more 'exploded' the view looks. Results are in file DomainDecomposition.000.vtu. The domains may be painted using the scalar variable `Domains` .

```
PlotList DomainDecomposition {
  Paraview
  TimeInterval 100. s
  ttL Tile {
    DomainDecomposition 1.3
  }
}
```

11.6.8 Summary of plotting options

A complete list of available options is shown below

```
PlotList 'Name' {
  ...
  ttL Block { ExternalCellFacets }
  ttL Block { Cells  MinimumCrackOpening 0.01 mm }
  ttL Block { CellOutline }
  ttL Block { Particles}
  ttL Block {
    FacetVariable 2
    // range parameters are specified after contour or facet
    // variable is selected and must have the units of the
    // variable
    RangeMinValue 5 psi
    RangeMaxValue 1000 in/s
    // facets outside range are not displayed unless
    [ DisplayAboveMax ] // facet above max are display in red
    [ DisplayBelowMin ] // facet below min are display in blue
```

```
  }
  ttL Block { SolidCells } // paraview only
  ttL Block { Slice } // quasar only
  ttL Block { DomainDecomposition 1.3 } // paraview only
```

11.6.9 Parallel processing with Paraview

The MARS plot generating procedures for Quasar and Paraview are very different. Quasar expects a single input file; as such, the contributions to each list from the various processes must be combined in MARS. Paraview can read and combine files generated from different processes. This eliminates the need to combine large data sets in rank zero process, which could lead to memory requirement problems. The Paraview files have the following name convention `'plotListName'.nnn.ppp.vtu`, where `nnn` is an integer represeting the sequential time frame and `ppp` is a three-digit integer representing the rank of the process that generated the file. In addition to these files, there is an additional file name `'plotListName'.pvd` that contains direction for Paraview on how to load and combine the previous files. This is one of the files that shows up in the Paraview Open window, and it is the one that should be selected.

11.6.10 Other examples

The following example shows the commands for generating facet contour plots of the inter-cell gaps for half of the model while eliminating the small fragments. (The elimination of the small fragments is optional.) The external faces of half of the tile are also generated in a separate list. The external faces are supposed to be displayed in gray or any neutral color, where the facets are to be displayed in color.

```
TetSolidList Tile {
  EditNodeList {
    Select cx > 0. in
    SaveSelectione HalfTile
    Select all
  }
}
PlotList ExtrnCells {
  TimeInterval 0.01 ms
  Paraview
  ttL Tile {
    ExtCellFaces
    MinimumFragmentMass 1.e-6 lb-s2/in
    LoadNodeSelection HalfTile
  }
}
PlotList Cntr {
  Paraview
  TimeInterval 0.01 ms
```

```
  ttL Tile {
    FacetVariable "Total crack opening"
    RangeMinValue 0.10 mm
    RangeMaxValue 0.3 mm
    DisplayAboveMax
    MinimumFragmentMass 1.e-6 lb-s2/in
    LoadNodeSelection HalfTile
    Scale 1000
  }
}
```

11.7 Embedded Fibers

Fibers of various types are used in construction materials to enhance durability, strength-to-weight ration, ductility, energy absorption capability, etc.In the context of LDPM, fibers-concrete interaction is explicitly modeled at the micro scale level by including the mechanical effect of fiber interaction at the facets where fiber-facet intersection occurs. The distribution of fiber-facet intersection is accomplished by generating distributions of fibers similar to actual distributions found in real specimens. From a geometric point of view, physical fibers can be described using few parameters: fiber density, length, diameter, and tortuosity. The latter parameter is used to characterize how bent fibers are: a straight fiber has no tortuosity while a fiber with many *kinks* is very tortuous. These geometric parameters are used in MARS for generating random fibers inside a control volume, which can either be the volume of the concrete part or a larger volume that contains the concrete part. Each fiber is model using a sequence of one or more segments linked together. Single segments are sufficient for generating straight fibers. Multiple segments are necessary for generating *tortuous* fibers. Fiber location and orientation is random. All fibers are completely contained in the control volume. For cast fiber-reinforced concrete parts, the control volume should be equal to the volume of the concrete part. For machined parts, the control volume should be larger than the part. The fibers that intersect the external surface of the part are treated as cut. The portion of a *cut* fiber which lays inside the part is shorter than the length of original fiber and this affects the mechanical characteristics of the fiber-facet interaction of the facets near the external surfaces. In the spirit of the discrete multi-scale physical character of the LDPM, the occurrences of fiber-facet intersections are determined by actually computing the locations where fibers cross inter-cell facets. This computation can require significant resources for large models in term of both time and memory. For this reason, an efficient bin-sorting algorithm was developed for computing these intersections. For each intersection, the lengths of the fiber on both sides of the facet and the angle at which the fiber intersects the facet are also computed. These parameters are saved in the facet data structure and used during the simulation for computing the incremental force effect of the fiber on the structural response of the concrete.

```
TetSolidList 'ListName' LDPM {
  . . .
```

```
  EmbeddedFibers {
    FiberConcreteInteraction 'ModelName'
    GenerateFibers {
      FiberLength 10. mm
      ElementSize  2. mm // Obsolete; use EdgesPerFiber
      EdgesPerFiber 5
      // Specify either fiber diameter, radius or area
      FiberDiameter 0.2 mm
      FiberRadius 0.1 mm
      FiberSectionArea 0.0314 mm2
      // Specify either NumberOfFibers or VolumeFraction
      NumberOfFibers 10000
      VolumeFraction 0.02
      Tortuosity 0.2
      Seed 345
      [ PreferentialDirection 'nx' 'ny' 'nz' 'scale' ] // [1]
      [ Chopped ]
      [ Prism ] // [2]
    }
  }
```

[1] This command is used when fibers are mostly oriented in a specific direction. The scale number is used to control how strong the orientation is. For a scale equal to 1., there is no preferential direction. For a scale equal to 10., a fiber is ten times more likely to be oriented in the given direction than to a direction orthogonal to it. The best way to set this parameter is to generate fiber distributions and compare them visually against available data.

The `GenerateFibers` command creates a new edge list automatically named `Fibers`. For this reason, it is important to avoid naming other edge lists with the word Fibers. This list can be later operated on using standrard procedures. For example:

```
TetSolidList 'ListName' LDPM {
  . . .
  EmbeddedFibers {
    GenerateFibers {
    . . .
  }
}
EdgeList Fibers {
  Rename 'SteelFibers'
  Write PartMeshDataFile 'fibers.mrs'
  Color red
}
```

[2] The `Prism` option was added in June 2012 to address some performance issues for models with large number (in the millions) of fibers. It is not a new parameter, rather

it is a flag to activate a new generation method. The default method uses the following procedure:

- Fibers are generated during the Reading phase and saved to an EdgeList named'Fibers'
- The generation method employs the tetrahedral mesh for ensuring that the fiber is entirely or partially contained in the concrete
- For chopped fibers the method finds the intersection of edges against the external facets of the tetrahedral mesh
- In the initialization phase, the fiber EdgeList is used for computing the intersection of the fibers themselves with the Ldpm facets.
- Fibers are not used as structural elements during the simulation

The procedure above works well for medium size fiber systems (less than a million). When the number of fibers is in the millions, the procedure is very slow because of all the check it has to perform. Furthermore, storing a large number of edges and nodes, which are not used in the calculation, wastes a significant amount of memory.

Since most of the FRHSC specimens so far encountered have a parallelepipedal shape and the edge list does not have to be stored, the new modified procedure can solve fiber-concrete interaction more effectively for prismatic geometries. The new procedure consists of:

- Fibers are temporarily generated during the initialization phase for the sole purpose of computing fiber-facet intersections
- The geometry is assumed to be a parallelepipedal prism aligned with the axis, this simplifies the computations of the edge locations and intersections with external surfaces,The logic is MPI parallelized: while all the processes generate exactly the same fibers based on the seed number, each process will consider only the fibers overlapping its domain.

Output for the new procedure appears in the initialization phase:

```
Initializing concrete-fiber interaction
  Number of fibers 53760
  Number of edge segments 191612
  Total fiber length     1.38e+3 m
  Fiber volume  327.69e-6 m2
  Number of fiber-facet intersections 526449
```

12 Hexahedral Solid Elements

The HexSolidList can be used to define a set of hexahedral 8-node solid elements. These elements can represent:

- purely geometric entities,
- deformable finite elements, or
- a set of disconnected rigid bricks.

The type of element is specified in the first line after the list name.

```
HexSolidList 'ListName' 'type' {
  // where the keyword 'type' can be one of the following:
  // Geometry: this can be used to define rigid bodies
  // Rigid: this is used to define separate bricks
  // FBSingleIP: Flanagan-Belitshcko formulation
  // 8IP: FE fomulation with 8 integration points
  // HyperElastic: formulation for rubber-materials
  // SimpleHex: simplified formulation for prismatic elements
  // Explosive: this employs EOS materials
  //
  // 1.) If this list is used to define a rigid body, enter
  Density 7.8 g/cm3
  // else
  Material MATE
  // You can also use
  InsertMaterial Mat {
    . . .
  }
  // when material was not previously defined
  // 2.) If mesh is explicitly defined enter
  NodeList Nodes
  // or
  InsertNodeList Nodes {
    . . .
  }
  ReadObjects 345 // number of elements
  //  i   n1   n2   n3   n4   n5   n6   n7   n8
      1  124  243   56  165  234  312   23  126
      2   56  238  121   78   56   98  126   66
      . . .
  // else, if mesh is internally generated, enter
  Generate {
    . . . // see below for generation options
```

```
  }
  // or
  SplitTetMesh 'tetMeshListName'
  // 3.) optional commands
  Make QuadFaceList 'ListName' // {2} generate a list of external surfaces
  Smooth
  Make TriangFaceList 'ListName'// {3} generate a list of external surfaces
  Make particleList PRTC { ... } // see below
  Make HexSolidList SLCT // make sublist of select hexes
  Make EdgeList 'ListName' AllEdges
  // make HexSolidList of selected elements
  Make HexSolidList ListName {1}
  Refine RFN6 // Refine mesh by splittying 2x2x2
  // select commands
  Select, Unselect, ... // see below
  RemoveUnselectedElements // {4}
  // to operate on the node list
  EditNodeList {
    . . . // nodelist commands
  }
  // use this command to save the mesh in a separate file
  Write PartMeshDataFile PART.mrs
  Write ElementDataFile PRT1.mrs  // elements only
  // use this command to read nodes and elements previously saved
  ReadFile PART.mrs
}
```

12.1 Select Commands

```
  Select [criterion]
  AlsoSelect [criterion]
  Unselect [criterion]
  Reselect [criteroin]
  InvertSelection
  [criterion] can take one of the following forms
    all    // all elements
    do 25  // element 25
    do 1 5 // elements 1 through 5
    do 1 100 2 // elements 1 through 100 step 2
    vl > 0.4 // elements with volume > 0.4
    vl = 0.4 // elements with volume apprx = 0.4
    vl < 0.4 // elements with volume < 0.4
    1n // elements with at least one node selected
    8n // elements with all eight nodes selected
Examples:
```

```
  Select do 1 100 // select element 1 through 100
  AlsoSelect do 201 300 // add elements 201 - 300
  Reselect 8n // select only element with all eight nodes
              // selected from elements selected above
```

Hex solid lists and all derived lists include commands for selecting nodes: 'SelectNodes', 'UnselectNodes', and 'ReselectNodes'. See examples in the NodeList section.

12.2 Generate Commands

These commands make it possible to generate hex meshes for simple parts within the MARS code. Multiple parts can be generated within a single list and possibly fused together by merging the overlapping nodes using the MergeParts command. The generate commands create a new list of nodes if necessary and appends the new nodes to the current list of nodes.

```
HexSolidList 'ListName' 'ListType' {
  . . .
  Generate {

    Cylinder {
      ReferenceSystem RFSY // cyl axis // z-axis
      Radius 4. in
      EdgesOnCircle 24 // must be multiple of 8
      Length 8. in
      ElementSize 1. in
    }

    Sphere {
      ReferenceSystem RFSY  // cyl axis // z-axis
      Radius 4. in // radius of cylinder
      EdgesOnCircle 40 // must be multiple of 8
      Translate 3. in 0. in 0. in
    }

    // rotate quad face list Q around z-axis of R for A degrees
    Rotate { Q SECT A 360 d 20 R CYLN }

    Extrude {
      QuadFaceList Disk
      Length 4 in
      ElementSize 0.4 in
    }

    wall { h 96 w 172 t 12 B }
```

```
    Block {
      ReferenceSystem RSYS
      Dimensions 4 in 8 in 20 in
      Elements  2 4 10
      Move 2. in 0. in 4. in
    }

    SuperBlock {
      LengthUnits cm
      // format  Dir crd1 elements1 crd2 elements2 crd3 ...
      X -8. 4 -2. 4 2. 4 8. 0
      Y -8. 4 -2. 4 2. 4 8. 0
      Z -8. 4 -2. 4 2. 4 8. 0
    }

    MergeParts 0.001 in
  }
}
```

12.3 Make Commands

1 The 'Make HexSolidList' is used for generating a sub-list of hex elements which have been selected. The new list is of the 'Geometric' type; in other word, MARS will not try to compute internal forces.

2 The 'Make QuadFaceList' is used for generating a list of all quadrilateral external surfaces of the complete mesh. If the user desires to generate external faces of a portion of the mesh, then the 'Make HexSolidList' command should be done first and the face list should be generated from inside the hex sub-list.

3 The 'Make TrianFaceList' is used for generating a list of triangular surfaces by splitting the quadrilateral faces of the list generated using the 'Make QuadFaceList' command. If the quad-face list was not previously generated, MARS will automatically generate it.

The 'Make EdgeList' command is used to generate a list of edges from the edges of the hexahedral elements. This command must be terminated by a keyword for the edge selection criterion; three options are available:

```
Make EdgeList 'ListName' AllEdges
Make EdgeList 'ListName' SurfaceEdges
Make EdgeList 'ListName' SharpEdges
```

The option 'AllEdges' is used to generate a list of all internal and external edges of the hex mesh. The other two options rely on the list of external quad faces generated using the 'Make QuadFaceList' command. If the quad-face list was not generated, MARS will automatically generate it. The option 'SurfaceEdges' is used to generate all external edges of the hex mesh. This list is useful for edge-edge contacts. The option 'SharpEdges' is used to generate a list of edges for which the attached faces form an angle greater than

60 degrees. This list is useful for graphics when we want to represent the outline of a solid component.

4 The option 'RemoveUnselectedElements' is used to permanently remove unselected elements from the list. This operation is done during the reading phase. It should be done before 'Make QuadFaceList' or 'Make EdgeList' for these derived list to be consistent with the reduced hex list.

12.4 Time History Commands

The following line commands are intended to be used inside `TimeHistoryList's` to produce records of global list variables or variables associated to a single element. Most of the variables are meaningful only for deformable hex elements. For element formulations where the requested variables are not available, the record will consists of zero values.

```
TimeHistoryList HIST {
  . . .
  // histories for entire list
  hxL-PART Volume            // [1]
  hxL-PART InternalWork      // [1]
  hxL-PART DissipatedEnergy  // [1]
  hxL-PART ElasticEnergy     // [1]
  hxL-PART HourglassWork     // [1]
  hxL-PART MaxVonMisesStress   // [2]
  hxL-PART MaxStateVariable 7  // [2]
  hxL-PART MinStateVariable 4  // [2]
  // histories for single element
  hx-PART 1 vl   // volume of element 1
  hx-PART 1 vm   // Von Mises stress
  hx-PART 1 pr   // pressure
  hx-PART 1 I1   // first invariant
  hx-PART 1 J2   // second invariant
  hx-PART 1 sv 3 // state variable 3
  hx-PART 1 xCG  // element x-coord of center of gravity
  hx-PART 1 yCG  // element y-coord of center of gravity
  hx-PART 1 zCG  // element z-coord of center of gravity
}
```

[1] These variable are computed taking the integral of a quantity over all elements in the list

[2] These variable are computed taking the maximum value (or minimum value) of a quantity over all elements in the list

12.5 Plot Attribute Commands

Plotting attributes can be specified in the element list or in the plot list

```
HexSolidList PART {
  . . .
  PlotAttributes {
    ContourVariable sv 1
    NoNodalAveraging
    NoSmoothing
  }
}
PlotList PLOT {
  . . .
  hxL SolidPart {
    // you may selecte one of the contour variables below
    ContourVariable StateVariable 1
    ContourVariable Velocity
    ContourVariable X-Velocity
    ContourVariable Y-Velocity
    ContourVariable Z-Velocity
    ContourVariable MinPrincipalStress
    ContourVariable MaxPrincipalStress
    ContourVariable VonMisesStress
    // stresses are averaged at the nodes unless ..
    NoNodalAveraging
    SelectedElementsOnly
    NoSmoothing  // discrete colored fringe plots
    // prescribe range after countour variables is selected
      (use appropriate units)
    RangeMinValue 0 psi
    RangeMaxValue 10000 psi
  }
  hxL PRT2 { OutlineOnly }
}
```

12.6 Particle Generation Commands

```
HexSolidList WALL {
  Material CNCR // mtCConcrete type
  // Enter or generate FE mesh
  . . .
  Make ParticleList PRTC {
    GapScalingFactor 0.05 // <gsf> min inter-particle
                          // gap > 0.05 x min aggr. diam (dfl=0.1)
    Seed 1543 // integer seed for random no. gener.
    PlotSieveCurve
    Debug
    ConstantSpacedParticlesOnEdges
```

```
  }
}
#-- if rebars are present in the model enter
  Make ParticleList PRTC { npL RBR1 npL RBR2 }
#-- where RBR1 and RBR2 are rebar slave particle lists
```

The 'Make ParticleList' is currently not working properly. An alternative particle generation method is executed using the command 'Make ParticleList2'. This method is intended to work with solid meshes where the external facets are used as external facets of the LDPM mesh. The mesh density should be controlled so that the external facets are of the correct dimensions. For example, a LDPM sphere can be generated using the following commands:

```
HexSolidList Ball Geometry {
  Material CONC
  Generate {
    Sphere {
      Radius 150 mm
      EdgesOnCircle 20
    }
  }
  Make ParticleList2 PRTC {
    seed 173521
  }
}
```

More specifically, MakeParticle2 follows the following logic: 1) find external quadrilateral faces of the hexahedral mesh, 2) split quadrilateral faces into triangular faces, 3) the triangular faces are passed to tetgen which uses them when generating the tetrahedral mesh, 4) generate a list of particles from largest to smallest, 5) insert each particle inside the volume of the solid using a random process (every point inside the volume has the same probabilty of being chosen independently of the size of the element that contains it), 6) if particle does not interfere with external surfaces or previous particles, fix its position, 7) once all particles have been placed, pass particle list to tetgen what will use them to anchor internal points of the triangular mesh.

12.7 Fragmentation Commands

```
#-- select one of the probability functions
  Weibull { . . . }
  Cracking { dmn 0.01 in efl 0.2 random fe 100 N/m }
#-- defaults dmn = 0.  efl = 0.
```

13 Rigid Bodies

A MARS rigid body consists of a set of nodes kinematically tied together. There are two main ways to select the nodes that form a rigid body: 1) within a node list, select all nodes or a subset of nodes and enter the node list for processing, 2) enter an element list for a specific mesh. As an example of the second way, let's say we want to convert a solid body (discretized using an hexahedral list) into a rigid body, we first need to define the solid using an HexSolidList specifying the density and not the material:

```
HexSolidsList 'HexListName' Geometry {
  Density 7.8 g/cm3
  NodeList 'NodeListName'
  . . .
  ReadObjects ...
  . . .
}
```

and then define the rigid body

```
RigidBody 'RigidBodyName' {
  HexSolidList 'HexListName'
}
```

In either case, the geometry and material density are used to computethe nodal masses. In turn, the nodal masses are used to compute the rigid body total mass and moment of intertia tensor.

Several types of objects can be tied together to form a rigid body. All nodes used to define these objects are enslaved to the translation and rotations of the master rigid body. Currently, the following lists can be used for the definition of a rigid body:

```
ndL, NodeList
hxL, HexSolidList
qfL, QuadFaceList
qsL, QuadShellList
tfL, TrngFaceList
tsL, TrngShellList
bmL, BeamList
eeL, EdgeList
ttL, TetSolidList
```

The rigid body initialization method automatically computes the total mass, center of gravity, and tensor of inertia of the rigid body based on the inertial properties of the components. These values can be overwritten using the following commands:

```
RigidBody 'BodyName' {
  . . .
  Set Mass 45.3 Kg
  ine  543 Kg.m2  34 Kg.m2  167 Kg.m2
  . . .
```

Boundary conditions and initial velocities imposed at the nodes of the original lists are disregarded. Boundary conditions and initial velocites can be imposed on the rigid body. The general input format for a rigid body is shown below:

```
RigidBody 'RigidBodyName' {
  // 1. enter a sequence of lists of objects that will be
  //    connected as a rigid body
  NodeList 'NodeListName'
  HexSolidList 'SolidListName'
  HexSolidList 'SolidListName'
  BeamList 'BeamListName'
  TriangShellList 'ShellListName'
  // 2. set boundary conditions (optional)
  Set Translations XXX
  Set Rotations XXX
  // 3. set initial velocities and/or rotation rates (optional)
  Set Velocities 15 in/s 0 in/s 0 in/s
  Set X-Velocity 15 in/s
  Set RotationRates 0. rad/s 0. rad/s 14. rad/s
  Set Z-RotationRates 14.
  // 4. overwrite calculated mass (optional)
  Set Mass 15 Kg
}
```

13.1 Time History Commands

The following line commands are intended to be used inside `TimeHistoryList's` to produce records of rigid body variables.

```
 TimeHistoryList Hist {
   . . .
   RB-'bodyName' vx // x-component of CG velocity
   RB-'bodyName' vy // y-component of CG velocity
   RB-'bodyName' vz // z-component of CG velocity
   RB-'bodyName' wx // x-component of rotation rate
   RB-'bodyName' wy // y-component of rotation rate
   RB-'bodyName' wz // z-component of rotation rate
   RB-'bodyName' cx // x-component of CG coordinate
   RB-'bodyName' cy // y-component of CG coordinate
   RB-'bodyName' cz // z-component of CG coordinate
   RB-'bodyName' fx // x-component of force
   RB-'bodyName' fy // y-component of force
   RB-'bodyName' fz // z-component of force
   RB-'bodyName' mx // x-component of moment
   RB-'bodyName' my // y-component of moment
   RB-'bodyName' mz // z-component of moment
```

14 Loadings

14.1 Nodal Load List

Use these commands to specify forces or moments to a single node, a set of nodes, or a rigid body. Loads vary in time according to the time history specified in the load curve.

```
NodalLoadList 'ListName' {
  // 1. Enter 'Moments' if you want to apply moments instead
  //    of forces (Opt.)
  Moments
  // 2. Enter either NodeList or RigidBody (Req.)
  NodeList 'NodeListName'
  RigidBody 'RigidBodyName'
  // 3. Enter LoadCurve (Req.)
  LoadCurve 'LoadCurveName'
  // 4. Enter load direction (Req.)
  Direction 0. 1. 0.
  // 5. Enter scaling factor (Opt.) and/or Distribute
  Scale -1.
  Distribute // [1]
  // 6. Use one of the four lines below to specify nodes
  //    (Required when NodeList is used)
  Node 1 // single node
  Nodes { 1 4 7 9 } // multiple nodes
  All // all nodes in the list
  SelectedNodes
  // Nodes can be selected inside this block using the
  // EditNodeList command
  EditNodeList {
    Select cx > 0.
  }
  SelectedNodes
}
```

[1] The `Distribute` command is used to distribute the load equally among the specified nodes. If this command is not used, each node will be loaded with the specified load. This requires requires

Alternate way

```
NodalLoadList 'ListName' {
  NodeList 'NodeListName'
  LoadCurve 'LoadCurveName'
  ReadObjects 2
  // nd  dx dy dz  scl
```

```
     54  1. 0. 0.  2.3
     58  1. 0. 0.  2.5
}
```

14.2 Prescribed Velocities List

Use these commands to specify velocities or rotatation rates to a single node, a set of nodes, or a rigid body. Velocities vary in time according to the time history specified in the load curve.

```
PrescribedVelocityList 'ListName' {
  // 1. Enter 'Rotations' if you want to apply rotations
  //    instead of velocities (Opt.)
  Rotations
  // 2. Enter either NodeList or RigidBody (Req.)
  NodeList 'NodeListName'
  RigidBody 'RigidBodyName'
  // 3. Enter LoadCurve (Req.)
  LoadCurve 'LoadCurveName'
  // 4. Enter load direction (Req.)
  Direction 0. 1. 0.
  // 5. Enter scaling factor (Opt.)
  Scale -1.
  // 6. Use one of the four lines below to specify nodes
  //    (Required when NodeList is used)
  Node 1 // single node
  Nodes { 1 4 7 9 } // multiple nodes
  All // all nodes in the list
  SelectedNodes
  // nodes can be selected inside this block using the EditNodeList command
  EditNodeList {
    Select cx > 0.
  }
  SelectedNodes
  // 7. Use line below for multiple orthogonal velocity constraints  DisregardMultipleC
}
```

Alternate way

```
PrescribedVelocityList 'ListName' {
  NodeList 'NodeListName'
  LoadCurve 'LoadCurveName'
  Input 2
  // nd  dx dy dz  scl
     54  1. 0. 0.  2.3
```

```
     58  1. 0. 0.  2.5
}
```

Rigid Body

```
PrescribedVelocityList 'ListName' {
  RigidBody 'RigidBodyName'
  LoadCurve 'LoadCurveName'
  Direction 0. 1. 0.
}
```

In general, you cannot impose multiple 'hard' constraints on the same node. For example, you cannot impose a prescribed velocity to a node which is part of rigid body. MARS flags nodes that have 'hard' constrained imposed on them. If you intend to impose multiple prescribed orthogonal velocity conditions on the same node, use the DisregardMultipleConstraints' keyword. keyword.

MPI. For the purpose of MPI parallelization, all processors impose velocities or rotations rates whether they own the nodes or not. This operation is computationally inexpensive and there would be no benefit in distributing it.

15 Constraints

Mars provides several types of constraints for modeling the interaction between different parts in a model. Constraints can be loosely divided into two categories: penalty formulations and master-slave formulations.

The penalty formulations are very reliable and do not create conflicts. They do however only approximate the actual constraint and in some cases the forces generated are not sufficient to enforce the constraints properly. Using stiff penalty parameters improves the effectiveness of the constraint but increasing the stiffness may eventually introduce local high frequency modes that require small time steps for stability. When using penalty formulations, the user should make sure that results are not dependent on the choice of the stiffness constants. This can be done by executing two or more simulations, doubling the stiffness each time. If results do not change appreciably between executions, then the stiffness is sufficient to enforce the constraints properly. The penalty forces are computed in the polymorphic method `calcFrc()`.

The master-slave formulations are very rigorous in enforcing constraints. However, there are many pitfalls in their usage. The main problems occur when multiple 'hard' conditions are applied to the same entities. These include rigid body lists, prescribed velocity lists, boundary conditions, and multiple master-slave constraints. When multiple 'hard' conditions are applied to the same nodes, results can be unpredictable. In most cases, Mars will write a warning message when multiple conditions are applied to the same node. If done properly, the results can be correct. It is important for the user to fully understand how constraints work and how they may interact with each other to avoid erroneous results. Master-slave constraints are enforced in two stages: a stage where the forces of the slave objects are transferred to the master objects implemented

in the polymorphic method `reduceFrc()`, and a stage where the velocities of the master objects are used to control the velocities of the slave objects implemented in method `applyKin()`. In the solver loop, they appear in this order

```
while (t < t_end) {
    for i = 1, 2, ... N-1, N
        list[i]->clearNodalForces()
    for i = 1, 2, ... N-1, N
        list[i]->calcFrc()
    for i = N, N-1, ... 2, 1
        list[i]->reduceFrc()
    for i = 1, 2, ... N-1, N
        list[i]->integrateEOM()
    for i = 1, 2, ... N-1, N
        list[i]->applyKin()
}
```

The user should note that when reducing the forces in the `reduceFrc` method, the lists are processed in the reverse order. This is very important when multiple constraints are imposed.

15.1 Node-Face Constraint List

```
TrngFaceNodeBondList BNDS {
  // abbreviated notations in < > brackets
  NodeList NODS  // <ndL NODS>
  FaceList FACS  // <tfL FACS>
  Tolerance 0.45 mm
  // constraint types
  // 2. Master slave, slave nodes may not lay on surface, rotation are not constrained
  MasterSlaveNoRotations
  // 3. Master slave, slave nodes may not lay on surface, rotation ARE constrained
  MasterSlaveWithRotations
  // 7. Master slave, slave nodes lay on surface, rotation are not constrained
  SlavesOnSurface
  // 6. Nodes slide over surface,
  SlidingWithFriction 0.3 0.2  0.1 mm // [1]
  // Enter lines below if bonds are entered explicitly
  num  345
  lst
  // j   jN   jF
     1  254  556
  . . .
  // 7. Mpi directives
  Mpi { OwnedByNodeOwner } // [2]
```

```
  Mpi { OwnedByFaceOwner } // default
}
```

[1] The sliding with friction constraint is designed to force a set of nodes to move over a surface. The constraint perpendicular to the surface is treated using a master-slave formulation. The resistance to sliding within the plane is treated with a stick-slip friction model. When the node is sliding, the friction factor f_f is computed using this expression

$$f_f = f_k + (f_s - f_k)\frac{A}{A+d}$$

where f_k is the kinematic friction factor, f_s is the static friction factor, A is a characteristic length (derived from fitting available test data), and d is the cumulative slip resulting from slippage computed during the simulation. The three parameters are specified in the command:

```
SlidingWithFriction 'sff' 'kff' 'A'
```

The node and the corresponding point on the surface *stick* together as long as the tangential inplane force F_t does not exceed the maximum friction force $F_{\max} = f_f F_n$, where F_n is the force normal to the surface. When F_t exceeds $F_{\max}$, the node starts slipping and the friction force is progressively reduced because of accumulated slippage according to the formula above. A constraint can return to the 'stick' status if tangential forces cannot maintain slipping. In this case, the cumulative slippage is NOT reset to zero. Warning: the current logic does not allow for a node to transition from one face to an adjacent face.

WARNING: this constraint uses a mixed formulation: the motion normal to the surface is imposed using master-slave constraints. It has not been possible to treat both formulation correctly and the internal forces in the perpendicular direction are not accounted properly. This algorithm may have some errors for high strain rates.

[2] In MPI executions, node-face constraints are distributed over the processors. Two options are available: 1) the processor that owns the face also owns the constraint, 2) the constraint is owned by the processor that owns the node. The first option is the default.

```
//   Fixed cylindrical surface
TrngFaceNodeBondList BNDS {
  NodeList NODS  // <ndL NODS>
  FixedCylSurface {
     ssm 0.0012
     csm 0.00015
     nsm 0.5 mm
     pnt 0. mm
     dir 0. 0. 1.
     rad 5 mm
     tol 0.0 mm
  }
}
```

The detection of the node-face pairs is automatically done. It is a good idea to check that the detection process found all the pairs. This is done in interactive mode by selecting

the contraint list and entering 'P' for plot at the `tbL>` prompt. This generates a plot file named `tbL.plt` that can be viewed with Quasar

15.2 Node-Tet Constraints

This constraint is used to tie a set of nodes to a corresponding set of points inside a tetrahedral element mesh. Each node and corresponding point share the same spatial location at time zero. Both penalty and master-slave formulations are available.

For the penalty formulation, there are three ways for computing the penalty stiffness:

1. constant stiffness for each constraint
2. stiffness computed based on time step and minimum node mass
3. stiffness computed using young's modulus of tet list material

If the stiffness is based on a time step, the following equation is used

$$K = \frac{m_{min}}{\Delta t^2}$$

where m min is the minimum mass of the five nodes participating in the constraint and Dt is the time interval specified via input. The smallest the time step, the larger the penalty stiffness resulting in smaller displacements. The idea is to select a time step close but slightly larger than the stable time step for the simulation.

If the penalty stiffnesss is based on the Young's modulis E of the material for the tetrahedral mesh, the penalty stiffness is computed using the equation

$$K = EV^{1/3}$$

where V is the volume of the element that contains point P corresponding to node N.

The input format for the penalty formulation is:

```
NodeTetConstraintList 'listName' Penalty {
  NodeList 'nodeListName'
  TetList 'tetListName'
  // choose one of the three options below
  ConstantStiffness 100 lbs/in
  StiffnessBasedOnTimeStep  0.001 ms
  StiffnessBasedOnYoungsModulus
}
```

If the master-slave formulation is used, the mass of slave nodes N is distributed to the nodes of the master tet element containing node N using the weighting factors computed from the shape functions. The input format for a master-slave formulation is:

```
NodeTetConstraintList 'listName' MasterSlave {
  NodeList 'nodeListName'
  TetList 'tetListName'
}
```

15.3 Node-Hex Constraints

This constraint is used to tie a set of nodes to a corresponding set of points inside an hexahedral element mesh. Each node and corresponding point share the same spatial location at time zero. Both penalty and master-slave formulations are available. The input commands for the penalty formulation are shown below:

```
NodeHexConstraintList 'listName' Penalty {
  NodeList 'listName'
  HexList 'listName'
}
```

The stiffness constant of a constraint between node N and point P is computed using this equation

$$K = EV^{1/3}$$

where E is the Young's modulus of the material for the hexahedral mesh and V is the volume of the element that contains point P corresponding to node N.

The input commands for the master-slave formulation are shown below:

```
NodeHexConstraintList 'listName' MasterSlave {
  NodeList 'listName'
  HexList 'listName'
}
```

The mass of slave nodes N is distributed to the nodes of the master hex element containing node N using the weighting factors computed from the shape functions.

15.4 Beam-Tet Constraints

The beam-tet constraint is designed to constrain the motion of strings of beam elements to the motion of a tetrahedral mesh. It is specifically intended to model rebar-concrete interaction, where concrete is modeled using a tetrahedral LDPM mesh. The node-tet constraint can be used for this purpose; however, the spacing of the constraints is dictated by the length of the beam finite elements. In the beam-tet constraints, we specify a number of points along each beam element and we enforce the constraint at all these points. The main obvious advantage of this formulation is that we can make the spacing of the constraints smaller than the average size of tetrahedral elements. In this way, the forces transmitted from the rebars are distributed in a smoother fashion to the concrete. A more significant advantage is the directionality provided by the beam elements. This makes is possible to model slippage in the axial direction, at least in the small deformation range. Three formulations are available:

- ElasticPenalty
- RebarConcreteInteraction
- RebarConcreteInteractionVE (volumetric effects)

15.4.1 Elastic formulation

This formulation ties a series of points along the beam element with corresponding points inside the concrete LDPM elements using penalty springs. The stiffnes of the penalty spring can either be computed based on a time step or defining a stiffness per unit surface. In the first case, the alogorithm finds the smallest mass m of the six nodes (two for the beam and 4 for the tet element) participating in the constraint and computes the stiffness using the formula K = m / (dt*dt)

```
BeamTetConstraintList 'listName' ElasticPenalty {
  BeamList 'beamListName'
  TetList 'tetListName'
  NumberOfConstraintsPerBeamElement 2
  Stiffness BasedOnTimeStep 0.002 ms
}
```

15.4.2 Elastic formulation with slippage

In this formulation, the beam element is assumed to be cylindrical, which is a good approximation for conventional rebars. A matrix of points is defined on the surface of the cylinder: n points in the axial direction and m points around the circumference. The corresponding points inside the tetrahedral mesh are also found. Each pair of rebar surface point and corresponding tet point forms a constraint. During the simulation, the constraint computes the components of the relative velocity between the two points in the local reference system: axial (along the beam axis), radial (perpendicular to the beam axis), and tangential (hoop direction). These three components are transfered to the rebar-concrete interaction (RCI) model, which is implemented as a `Material` class. The RCI model returns the three componenets of the stress vector in the local reference system, which are then used to compute forces at the beam and tet nodes.

```
BeamTetConstraintList 'listName' RebarConcreteInteraction {
  BeamList 'beamListName'
  TetList 'tetListName'
  NumberOfCircumferentialConstraintsPerBeamElement 3
  NumberOfAxialConstraintsPerBeamElement 2
  RebarRadius 10 mm
  Material 'RciModelName'
}
```

15.4.3 Elastic formulation with slippage and volumetric effects

This formulation has not been implemented at this time. When implemented, in addition to the relative velocity vector, a volumetric expansion term is also passed to the RCI model. The model returns a velocity vector as well as a pressure term which is applied to the tetrahedral element.

```
BeamTetConstraintList 'listName' RebarConcreteInteractionVE {
  BeamList 'beamListName'
  TetList 'tetListName'
  NumberOfCircumferentialConstraintsPerBeamElement 3
  NumberOfAxialConstraintsPerBeamElement 2
  RebarRadius 10 mm
  Material 'RciModelName'
}
```

15.5 Beam-Hex Constraints

15.5.1 Elastic formulation

```
BeamHexConstraintList NAME ElasticPenalty {
  BeamList RBRS
  HexList CNCR
  Stiffness BasedOnTimeStep 0.002 ms
}
```

15.5.2 Elastic formulation with slippage

```
BeamHexConstraintList NAME RebarConcreteInteraction {
  BeamList RBRS
  HexList CNCR
  NumberOfCircumferentialConstraintsPerBeamElement 3
  NumberOfAxialConstraintsPerBeamElement 2
  RebarRadius 10 mm
  Material INTR
}
```

15.5.3 Elastic formulation with slippage and volumetric effects

```
BeamHexConstraintList NAME RebarConcreteInteractionVE {
  BeamList RBRS
  HexList CNCR
  NumberOfAxialConstraintsPerBeamElement 2
  RebarRadius 10 mm
  Material INTR
}
```

15.6 Constraint List

This list includes a variety of miscellaneous constraints. It is somewhat different than other lists in the sense that it can group objects that are non-homogenous. It was done that way because there are many possible ways constraints can be formulated and it

seemed that there would be a proliferation of lists if every type of constraint would be given its own list.

```
ConstraintList 'ListName' {
   SlaveNodeMasterNodesConstraint { ... }
   SlaveNodeMasterNodeConstraints { ... }
   SlaveRigidBodyMasterNodeConstraint { ... }
   SlaveNodeMasterEdgeConstraint { ... }
   SlaveRigidBodyMasterEdgeConstraint { ... }
   NodeNodePenaltyConstraint { ... }
   HingePenaltyConstraint { ... }
}
```

15.6.1 Slave Node - Master Node Constraint

This list is designed to create a series of master-slave constraints that tie overlapping nodes from different lists. One list is the master list and the other is the slave list. A tolerance must be provided. The tolerance should be a very small length, such that the distance of the overlapping nodes is less than the tolerance. Optionally, only the translational degrees of freedom can be constrainded, while the two nodes can rotate independently.

```
ContraintList 'ListName' {
  SlaveNodeMasterNodeConstraints {
    SlaveNodeList 'ListName'
    MasterNodeList 'ListName'
    Tolerance 1. mm
    [ TranslationsOnly ]
    [ Debug ]
  }
}
```

15.6.2 Slave Rigid Body - Master Node Constraint

* * * T O B E I M P L E M E N T E D * * *

This constraint is designed to constrain a slave rigid body to translate with and/or rotate around a master node.

```
  SlaveRigidBodyMasterNodeConstraint {
    RigidBody 'RigidBodyName'
    MasterNode 'NodeListName' cl 5. cm 2. cm 5. cm
    Set Translations XXX  // constrained translations
    Set Rotations OOO    // free rotations
  }
```

15.6.3 Slave Node - Master Nodes Constraint

This constraint is designed to constrain a slave node from one node list to a set of nodes from another list. The master nodes are the nodes that lay in a sphere centered at the slave node with a given radius. The slave node is tied to move with the average velocity of the master nodes.

```
  SlaveNodeMasterNodesConstraint {
    SlaveNode 'NodeListName' 14
    MasterNodeList 'NodeListName'
    Radius 5.
  }
```

15.6.4 Slave Node - Master Edge Constraint

This type of constraint ties a node to a point on an edge. The constraint is of the master-slave type. The constraint interpolates coordinates, velocities, and rotations of the slave node. Rotation constrains can be disabled to simulate a spherical bearing. Alternatively only the rotation along the edge can be free to simulate a wheel spinning on an axle. MARS searches automatically for constraints: the nodes of a node-list that are within a given tolerance from the edges of an edge-list are constrained.

```
ConstraintList 'ListName' {
  SlaveNodeMasterEdgeConstraint {
    NodeList 'ListName'
    EdgeList 'ListName'
    Tolerance 1. mm
    [ FreeRotations ]
    [ AxialSpinning ]
  }
}
```

15.6.5 Slave Rigid Body - Master Edge Constraint

This type of constraint ties the center of a rigid body to a point on an edge. The constraint is of the master-slave type. The constraint interpolates coordinates, velocities, and rotations of the slave rigidbody. Rotation constrains can be disabled to simulate a spherical bearing. Alternatively only the rotation along the edge can be free to simulate a wheel spinning on an axle. MARS searches automatically for constraints: the edge that contains the rigid body within a given tolerance is used as master edge.

```
ContraintList 'ListName' {
  SlaveRigidBodyMasterNodeConstraint {
    RigidBody 'RigidBodyName'
    EdgeList 'ListName'
    Tolerance 1. mm
```

```
    [ FreeRotations ]
    [ AxialSpinning ]
  }
}
```

15.6.6 Node - Node Penalty Constraint

This type of constraint ties selected degrees of freedom of two nodes. The two nodes are supposed to overlap at time 0. For pratical purposes, a tolerance is specified via input and the distance between the two nodes must be less than the tolerance. The penalty forces are computed incrementally using velocities, e.g.:

$$F_x(t+dt) = F(x) + K(v_{xI} - v_{xJ})dt$$

where K is the penalty spring stiffness

```
ConstraintList 'ListName' {
  NodeNodePenaltyConstraint {
    // 1. select first  node
    Node 'ListName' 'nodeIndex'
    // or
    Node 'ListName' cl 5 cm 0. cm 8 cm.
    // 2. select second node
    Node 'ListName' 'nodeIndex'
    // or
    Node 'ListName' cl 5 cm 0. cm 8 cm.
    // 3. Enter penalty spring stiffness
    Stiffness 1.4e8 dyn/cm
    // 4.  Enter tolerance
    Tolerance 1. mm // [1]
    // 5.  Select one of the
    Translations XXX
    Rotations OOO
  }
}
```

This type of constraint ties selected degrees of freedom of two nodes to move together. together.

15.6.7 Hinge Penalty Constraint

This type of constraint ties two nodes so that they can rotate around a corotational axis. The two nodes are supposed to overlap at time 0. For pratical purposes, a tolerance is specified via input and the distance between the two nodes must be less than the tolerance. The penalty forces are computed incrementally using velocities. The hinge direction rotates with the average rotation rate of the two nodes

```
ConstraintList 'ListName' {
```

```
  HingePenaltyConstraint {
    // 1. select first  node
    Node 'ListName' 'nodeIndex'
    // or
    Node 'ListName' cl 5 cm 0. cm 8 cm.
    // 2. select second node
    Node 'ListName' 'nodeIndex'
    // or
    Node 'ListName' cl 5 cm 0. cm 8 cm.
    // 3. Enter penalty spring stiffness
    Stiffness 1.4e8 dyn/cm
    // 4.  Enter tolerance
    Tolerance 1. mm // [1]
    // 5.  Enter hinge axis direction
    HingeAxis 0.1 0.3 0.
    // 6.  Enter axial motion flag [optional, def = false]
    AxialMotion true
  }
}
```

This constraint make sense for nodes that have rotations

15.7 Particle-Rebar Interaction List

The particle-rebar interaction list is intended to couple rebar embedded in concrete LDPM regions. The input consists of the list of nodes which are used for defining the LDPM region and the list of rebar elements. The concrete-rebar interaction model is entered as a 'Material'. Note that ... The rebar radius must be explicitely entered.

The constraint detection phase identifies pairs of particles and rebar finite elements that interact with each other. This operation is performed once at the beginning of a simulation. The particle-rebar interaction constraint is then applied to each pair. Currently, we select all particles that are suitably close to the rebar elements. More specifically, we do not include particles whose spherical volume overlaps the cylindrical volume occupied by the rebars. We do include however, particles when their gap from the rebar is within a range specified by the analyst using the 'MinimumGap' and 'MaximumGap' commands. The rebar overlapping particles are connected to the other particles as if the rebar does not exist. Their effect is accounted for in the bond parameters when parameter calibration is performed.

The constraint formulation ties a single particle to a single beam element defined by its two nodes. The formulation consists of two parts: a kinematics part where the local deformation state is computed from particle/node velocities and rotations, a force reduction part where local stresses are used to compute forces and moments at the particle and beam nodes. nodes.

```
ParticleRebarInteractionList Constraints {
```

```
  NodeList Particles
  BeamList Rebars
  Material ConcRebarInt
  RebarRadius 0.6 cm
  MinimumGap 0.1 cm
  MaximumGap 2.0 cm
  EquilibratedAreas // opt
}
```

15.8 Particle-Fiber Interaction List

The particle-rebar interaction list is intended to couple rebar embedded in concrete LDPM regions. The input consists of the list of nodes which are used for defining the LDPM region and the list of rebar elements. The concrete-rebar interaction model is entered as a 'Material'. Note that ... The rebar radius must be explicitely entered.

The constraint detection phase identifies pairs of particles and rebar finite elements that interact with each other. This operation is performed once at the beginning of a simulation. The particle-rebar interaction constraint is then applied to each pair. Currently, we select all particles that are suitably close to the rebar elements. More specifically, we do not include particles whose spherical volume overlaps the cylindrical volume occupied by the rebars. We do include however, particles when their gap from the rebar is within a range specified by the analyst using the 'MinimumGap' and 'MaximumGap' commands. The rebar overlapping particles are connected to the other particles as if the rebar does not exist. Their effect is accounted for in the bond parameters when parameter calibration is performed.

The constraint formulation ties a single particle to a single beam element defined by its two nodes. The formulation consists of two parts: a kinematics part where the local deformation state is computed from particle/node velocities and rotations, a force reduction part where local stresses are used to compute forces and moments at the particle and beam nodes. nodes.

```
ParticleFiberInteractionList Constraints {
  NodeList Particles
  BeamList Fibers
  Material ConcFiberInt
  FiberRadius 0.6 cm
  MinimumGap 0.1 cm
  MaximumGap 2.0 cm
  Verbose // [1]
  // Use either 'EquilibratedArea' or 'TiledAreas'
  EquilibratedAreas // [2]
  TiledAreas 24 // [3]
  ProjectedNormalAreas
  DisableInternalFacets // [4]
}
```

[1] The `Verbose` command should be used only for small problems and is intended for debugging purposes. When 'Verbose' is entered, Mars will print a detailed status of all the particles interacting with each of the fiber elements. elements.

[2] The `EquilibratedArea` command is used for computing the interaction areas using the criteria described in the notes.

[3] The `TiledAreas` command computes interaction areas by subdividing the cylindrical surface of the fiber/rebar into tiles in the axial and cylindrical direction. Each area is assigned to one of the particle-edge contraints. The integer following the keyword indicates the number of areas in the hoop direction. The number of areas in the axial directions is computed by using the equation:

[4] The `DisableInternalFacets` is an optional command for disabling the LDPM facets whose centers lay inside the cylindrical volume of the fibers. These facets will not contribute any internal force.

$$n_A = L/(2\pi R/n_H$$

where R is the fiber radius, L is element length, and n_H is the number of circumferential areas specified above via input.

Warning: If an element is partially embedded in concrete, Mars distributes its whole surface areas to the particles interacting with that element. On the 'to do' list, there is the action item for computing what portion of a partially embedded fiber element is inside the concrete. If fibers are entirely embedded in concrete, this current formulation is adequate. For single fiber pull-out tests, subdivide a fiber so that there are no elements that are partially embedded: in other words, a node of the fiber sequence should just be slightly outside the concrete surface.

15.9 Bolt List

```
BoltList BLTS {
#-- abbreviated notations in < > brackets
  Material STEL
  Diameter 0.3 in
  StemLength 1.0 in
  BeamInStem 4
  HeadThickness 0.2 in
  HeadDiameter 0.6 in
#-- if bolts are entered explicitly
  num  345
  LengthUnits in
  lst
  // c0x, c0y c0z: origin of the stem
  // len: length of the stem
  // dcx, dcy, dcz: direction of the stem
  // n: number of beam elements along the stem
  // j   c0x  c0y  c0z  len  dcx  dcy  dcz   n
     1   0.0  10.   1.  0.6   1.   0.   0.   3
  . . .
```

```
}
```

16 Contacts

16.1 Contact Models

Contact models are employed by the contact formulations (e.g. node-face, node-node, edge-edge, etc) to compute contact forces based on the relative velocity of the material points associated to the two objects at the point of contact. Contact models have the same function as material models have in element formulations. Contact model commands are embedded in the contact lists (see examples)

16.1.1 Penalty contact model

The penalty-function contact model provides the simplest method for computing the normal contact force Fn as a function of penetration p. The method requires a single parameter, the stiffness Kl of the linear spring used in the equation. As an alternate way of computing stiffness, a time step may be entered. This time step is used in conjunction with the smallest mass of the nodes participating in the contact to define the penalty spring stiffness.

```
Fn = K * p.
```

The input commands can be enter either in a single line

```
ContactModel Penalty { Kl 1e6 N/m }
ContactModel Penalty { dt 0.001 ms }
```

or in multiple lines

```
ContactModel Penalty {
  SpringStiffness 1.e6 N/m
}
ContactModel Penalty {
  StiffnessBasedOnTimeStepOf 0.001 ms // [1]
}
```

[1] The smaller the time step, the stiffer the penalty springs are. One can check the amount of maximum penetration using time history commands in the contact lists.

ContactForce PenaltyEP

16.1.2 Penalty-hysteresys contact model

The penalty-function with hysteresis contact model provides the capability of modeling non-elastic contacts, where some energy is dissipated. This is accomplished by using different paths for loading and unloading. The initial loading follows a linear force-penetration relationship

```
Fn = K * p.
```

Unloading follows a different relationship

```
Fn =  C * p^b
```

where b is a non-dimensional parameter which is greater or equal 1,

```
C = FX / pX^b is constant,
pX is the penetration when unloading begins,
FX is the contact force when unloading begins.
```

For b=1 the unloading curve is the same as the loading curve and there is no hysteresis. For b=2, the unloading curve is a parabolic curve with apex at the origin and intersecting point (pX, FX). The area between the loading and unloading curve represents the energy dissipated in the loading-unloading event. The larger the value of b, the more energy is dissipated.

Reloading during the unloading phase is ruled by a special relationship. Reloading follows a steeper line, with the stiffness constant defined as the tangent to the unloading curve at pX

```
Fn = Kr * (p - pY)
```

where pY is the penetration when reloading begins, begins,

```
Kr = b * C * pX^(b-1) is the stiffness
```

The normal force Fn cannot exceed Fn = K * p value; in other words, the initial loading curve acts as an upper envelope.

The input commands are either

```
  ContactForce PenaltyHyst { Kl 1e6 N/m [ Beta 3 ] }
or
  ContactForce PenaltyHyst {
    LinearSpring 1.e6 N/m
    [ Beta 3. ]
  }
```

16.1.3 Hertz contact model

The Herz contact force computes the normal contact force Fn as a function of penetration using the well known equation

```
Fn = H p^1.5
```

The constant H is typically defined as a function of Young's modulus E and Poisson's ratio pr

```
H = 2/3 * E / (1-pr^2).
```

The input commands can be enter either in this format

```
  ContactModel Hertz { E 29e6 psi pr 0.3 }
or
  ContactModel Hertz {
    YoungsModulus 29e6 psi
    PoissonsRatio 0.3
  }
```

ContactForce HertzTU

16.1.4 Hertz-hysteresis contact model

The Hertz with hysteresis contact model provides the capability of modeling non-elastic contacts, where some energy is dissipated. This is accomplished by using different paths for loading and unloading. The initial loading follows the conventional Hertz relationship

```
Fn = H * p^1.5.
```

Unloading follows a different relationship

```
Fn =  C * p^b
```

where b is a non-dimensional parameter which is greater or equal 1.5,

```
C = FX / pX^b is constant,
pX is the penetration when unloading begins,
FX is the contact force when unloading begins.
```

For b=1.5 the unloading curve is the same as the loading curve and there is no hysteresis. For b=2, the unloading curve is a parabolic curve with apex at the origin and intersecting point (pX, FX). The area between the loading and unloading curve represents the energy dissipated in the loading-unloading event. The larger the value of b, the more energy is dissipated. A default value of 3 is used when no value of b is entered.

Reloading during the unloading phase is ruled by a special relationship. Reloading follows a steeper line, with the stiffness constant defined as the tangent to the unloading curve at pX

$$F_n = K_r(p - p_Y)$$

where p_Y is the penetration when reloading begins, begins,

```
Kr = b * C * pX^(b-1) is the stiffness
```

The normal force F_n cannot exceed the $F_n = Hp^{1.5}$ value; in other words, the initial loading curve acts as an upper envelope.

The input commands can be enter either in this format

```
ContactModel HertzHyst { E 29e6 psi  pr 0.3  beta 3}
```

or

```
ContactModel HertzHyst {
  YoungsModulus 29e6 psi
  PoissonsRatio 0.3
  Beta 3.
}
```

16.1.5 Stick-slip friction model

The 'stick-slip' friction model is an algorithm designed for computing tangential contact forces between two objects perpendicular to the normal direction at the point of contact. The tangential force is computed incrementally based on the tangential relative motion of the two objects at the point of contact and a penalty stiffness parameter. The tangential force is limited either by the static friction force if the objects are sticking, or the kinetic friction force if the objects are slipping. When the objects are sticking and the tangential force exceed the static friction force, the contact is assumed to convert from sticking to slipping. When the objects are slipping and the tangential force becomes smaller than the kinetic friction force, the contact is assumed to convert from slipping to sticking. The static friction force is defined as

```
Fsf = sfc * Fn

Fsf = sfc * Fn

Fkf = kfc * Fn
```

where sfc is the static friction factor coefficient and Fn is the normal contact force independently computed in one of the contact models described above. The kinematic friction force is defined as where kfc is the kinetic friction factor coefficient. kfc is typically less or equal than sfc. The input commands for the friction force model are:

```
FrictionForce { dt 0.01 ms sf 0.3 df 0.2 }
// or
FrictionForce {
  PenaltyStiffness 10 N/m //  short notation: K
  StaticFriction 0.3  //  short notation: sf
  DynamicFriction 0.3 // short notation: df
  StribeckVelocity 10 m/s
```

```
    dt 0.001 ms // for computing stiffness
    Beta 3.
    MinNormalForce 10. nN at 2 nm // f0 10. N
  }
```

The 'StribeckVelocity' is an optional parameter. If entered, the kinetic friction force is computed using the equation below below

```
  Fkf = (kfc + (sfc-kfc)*exp(-R^2)) * Fn
where  R = |dv| / Vs,
       |dv| is the norm of the relative tangential slipping velocity
       Vs is the Stribeck velocity
```

The parameter 'Beta' is optional and is used to 'kill' small residual elastic oscillations in the elastic range when the particles are sticking in a quasi motioneless equlibrium state. The dampening mechanism is not viscous (velocity-dependent) but hysteretic (based on cycle amplitude). For 'Beta' = 1., there is no hysteretic effect. Oscillation dampening increases as Beta increases. Beta must be greater or equal 1. The default value is 2 to provide some damping.

The 'MinNormalForce' is an optional parameter intended to approximate the effects of 'bonding forces' which oppose tangential motion even when the particles are not pressed against each other. The last parameter in the line, is the maximum gap for this effect to be included. The minimum normal force, f0, is added to the normal force when the particles are still sticking and the gap is less than the maximum gap. This virtual normal force increment results in a larger maximum static friction force. f0 is no longer added to the normal force when the particles start slipping thus simulating a failure in the bonding force. In the current formulation, f0 is added to the normal force when the slipping flag is false; thus, if slipping stops, the bonding force is re-established. Note that the actual normal force used in the computation of the contact force is not affected. The default value of f0 is 0. 0.

The parameter 'dt' can be used for computing the penalty spring stiffness as an alterative to the 'PenaltyStiffness' parameter. When 'dt' is selected, the value of the penalty stiffness for each contact is computed using the equation

```
K = 0.5 * ms / (dt*dt)
```

where ms is the minimum mass of any node/particle participating in the contact

16.1.6 Tangential elasto-plastic model

The tangential elasto-plastic model is an algorithm designed for computing tangential contact forces between two objects, in the direction perpendicular to the normal at the point of contact. The tangential force is computed incrementally based on the tangential relative motion of the two objects at the point of contact and a penalty stiffness parameter. The tangential force is limited by a 'maximum allowable force' fmx specified via input, using a predictor-corrector approach. When the predictor exceeds fmx, the

tangential force is scaled down to fmx and slipping between the surfaces occurs. The tangential force is computed only for surfaces with a gap smaller then a prescribed maximum gap gmx. This logic is summarized in the following pseudo-code

```
if (gap < gmx)
    ftn += K * dv * dt   // increment forces
    if (|ftn| > fmx)
        ftn *= fmx / |ftn|  // scale forces
else
    ftn = 0
```

The input commands are

```
TangentialPlasticForce {
  PenaltyStiffness 10 N/m //  short notation: K
  BoundingForce 10. nN
  MaximumGap 2 nm
}
```

The 'PenaltyStiffness' parameter is somewhat arbitrary. Physically, it represents the small local tangential deformations that take place when shear forces are present. In some configurations, like discrete particle models, the tangential penalty stiffness may affect the overall elastic stiffness of the system. This may be relevant in the small deformation range. However, the plastic behavior should not be affected significantly. The best way to assess how sensitive results are to this parameter is to run the same case with different values of the parameter.

The 'MinNormalForce' is an optional parameter intended to approximate the effects of 'bonding forces' which oppose tangential motion even when the particles are not pressed against each other. The last parameter in the line, is the maximum gap for this effect to be included. The minimum normal force, f0, is added to the normal force when the particles are still sticking and the gap is less than the maximum gap. This virtual normal force increment results in a larger maximum static friction force. f0 is no longer added to the normal force when the particles start slipping thus simulating a failure in the bonding force. In the current formulation, f0 is added to the normal force when the slipping flag is false; thus, if slipping stops, the bonding force is re-established. Note that the actual normal force used in the computation of the contact force is not affected. The default value of f0 is 0. 0.

The parameter 'dt' can be used for computing the penalty spring stiffness as an alterative to the 'PenaltyStiffness' parameter. When 'dt' is selected, the value of the penalty stiffness for each contact is computed using the equation

The parameter 'dt' can be used for computing the penalty spring stiffness as an alterative to the 'PenaltyStiffness' parameter. When 'dt' is selected, the value of the penalty stiffness for each contact is computed using the equation

```
K = 0.5 * ms / (dt*dt)
```

16.1.7 Rolling resistance model

Rolling resistance is the resistance to rotational motion that occurs when two objects roll over each other. Rolling resistance is caused by local deformations in one or both of the objects in contact. Strictly speaking, the rolling resistance is defined as a force that opposes the rolling motion of a round object over a flat surface. In MARS, the term 'rolling resistance' is used in a more general way, where we consider the relative rotational motion of two objects in contact. The relative rotational motion is opposed by equal and opposite moments applied on the two objects. The relative rotational motion is divided into two components: rolling and spinning, where spinning is aligned with the direction parallel to the contact normal direction and rolling is perpendicular to it.

MARS implemente rolling/spinning resistance with an algorithm similar to the tangential friction force algorithm. For the rolling component, a resisting rolling moment Mr is computed by integrating the relative rolling motion dwr of the two objects multiplied by a penalty stiffness constant Kr:

```
Mr = Int (Kr * dwr)
```

Mr is limited by the maximum allowable rolling moment Xr which is defined as

```
Xr = fr * L * Fn
```

where fr is a 'friction' coefficient provided via input, L is a characteristic length computed by the contact formulation (see below), and Fn is the normal contact force. For nanoparticle interaction L is the distance between the particle centers; for sphere-face contacts L is the distance between the center of the ispherical particle/node and the midplane of the face. face.

The spinning component (or twist) is treated in a similar fashion but its parameters are defined independently.

```
RollingResistance { Kr .. Kt .. Fr .. Ft .. Beta .. dt .. }
// or
RollingResistance {
  RollingStiffness ..
  TwistStiffness  ..
  RollingFrictionFactor  ..
  TwistFrictionFactor  ..
  dt ..
  Beta ..
  MinNormalForce 10. nN at 2 nm // f0 10. N
}
```

The optional parameter Beta provides a certain degree of hysteretic damping for small residual oscillations and works similar to the Beta in the friction force algorithm. No damping for Beta = 1, progressively more damping for larger beta's; default is beta = 2.

The 'MinNormalForce' is an optional parameter intended to approximate the effects of 'bonding forces' which oppose diffferences in rotation rates even when the particles are

not pressed against each other. The minimum normal force, f0, is added to the normal force resulting in a larger value for the maximum allowable rolling moment

```
Xr = fr * L * (Fn + f0).
```

The parameter 'dt' can be used for computing the penalty spring stiffnesss as an alterative to the 'RollingStiffness' and 'TwistStiffness' parameters. When 'dt' is selected, the value of the penalty stiffness for each contact is computed using the equation

```
K = 0.5 * rm / (dt*dt)
```

where rm is the minimum rotational mass (moment of inertia) of any node/particle participating in the contact

In the current version, the stiffness parameters are entered with no units, which makes this portion of the input, unit dependent. This will be corrected in future versions.

The MARS rolling resistance algorithm works in conjunction with the friction force algorithm to reproduce the resistive forces implied in the conventional definition of 'rolling resistance'. For example, the rolling resistance Fr (which is a force in the conventional definition) of an ordinary car tire on sand is approximately 0.3 time its weight W

```
Fr = 0.3 * W.
```

In MARS, this force is obtained by excercising both friction and rolling resistance models. The rolling resistance algorithm applies a resistive moment to the wheel equal to

```
Mr = 0.3 * Rw * W
```

This moment tends to reduce the wheel rotation rate and this in turn increase the tangential force at the wheel to a force of Ft = 0.3 * W, which is the rolling resistance force given by the conventional definition. The static and kinetic friction coefficients must be at least 0.3 in the MARS friction model for this to work. [The above discussion does not take into acount the rotational inertia of the tire.] Note however, that the MARS approach is capable or modeling not only the case of a tire rolling over sand with no apparent slippage, but also the more general cases where a tire slips on sand.

16.2 Node-Node Contact List

The node contact makes it possible to detect contacts between nodes/particles from a single node-list or two node-lists. For the purpose of contact, a dimensionless node takes a spherical shape. Contact begins when the external spherical surfaces of two nodes/particles start penetrating each other.

```
NodeNodeContactList 'ContacListName' {
  // variables with the % sign inherit defaults from control parameters
  // 1. Define node/particle lists
  NodeList 'FirstNodeListName'
```

```
  NodeList 'SecondNodeListName'
  // 2. Specify optional dimension controls
  Node1Thickness 0.4 cm // %
  Node2Thickness 0.2 cm // %  // if nodes are particles, node thickness is the larger o
  // select one of the three contact methods
  DetectionDistance 0.6 cm  // %
  // 3. Enter contact models, see previous sections
  ContactForce PenaltyHyst { . . . }
  FrictionForce { . . . }
  RollingResistance { . . . }
  UpdateInterval 0.000010 s // %
  Debug 6
}
```

When two node-lists are defined, then contact conditions are detected between nodes from the first list and nodes from the seconds list, but not between nodes within the same list. If contacts have to be detected between nodes/particles which belong to a single list, then only one 'NodeList' must be specified. For example, if we have two particles lists, red particles and blue particles and we want to be able to detect contacts between all particles independently of color, we need three contact lists

```
NodeNodeContactList BlueRedContacts {
  NodeList BlueParticles
  NodeList RedParticles
  . . .
}
NodeNodeContactList BlueOnlyContacts {
  NodeList BlueParticles
  . . .
}
NodeNodeContactList RedOnlyContacts {
  NodeList RedParticles
  . . .
}
```

There are some rules regarding the size of the nodes and particles. If one of the node-lists consists of spherical particles with finite radii, there is no need to specify a 'NodeThickness' for that list. However, if a 'NodeThickness is specified, MARS will take the larger value between the actual particle radius and the NodeThickness parameter. If the node thickness is not specified and the node-list consists of point-like nodes, then their radius is zero. Contact can be enforced as long as the other list has spherical nodes with finite radii. It is not possible to enforce contact conditions between two nodes, both of which have zero radii.

```
NodeNodeContactList GRNL {
```

```
  GranuleList GRNS
  . . .
}
```

16.2.1 Time Histories

The variables 'X-Force', 'Y-Force', and 'Z-Force' produce the sum of all contact forces in each direction. The variable 'NumberOfContacts' gives the total number of potential contacts being monitored. The variable 'NumberOfActiveContacts' gives the number of nodes that are actually in contact.

```
TimeHistoryList 'ListName' {
  . . .
  ncL-'ListName' X-Force
  ncL-'ListName' Y-Force
  ncL-'ListName' Z-Force
  ncL-'ListName' InternalWork
  ncL-'ListName' NumberOfContacts
  ncL-'ListName' NumberOfActiveContacts
}
```

16.3 Edge Contact List

The edge-edge contact makes it possible to enforce contact conditions between edges, either from the same list or from two different lists. For the purpose of contact, an edge takes a three dimensional shape consisting of a cylinder capped by two hemispherical surfaces, the shape of some commonly found pills. The hemispherical surfaces are centered at the two nodes defining the edge. The radius of the cylinder and hemispherical surfaces is either provided by the edge lists or defined via input. Contact between two edges begins when the exernal surfaces of the associated 3-D shapes start penetrating each other. It is possible that in some cases, edges cut across each other. Here are some scenarios:

- The edges are thin (small radii) and the maximum contact force that can be generated ($F_{n,max} = K(r_1 + r_2)$) is less than the contact force required to prevent crossing. Remedy: increase penalty stiffness.
- The relative velocity of the edges is so large and the time step so coarse, that the contact algorithm does not have a chance to work. Remedy: reduce time step.

Although it would be possible to insert logic in the code to detect this scenarios, the computational cost would be considerable. It make more sense for the user to be aware

..

The input commands for the edge-edge contact list take the format

```
EdgeEdgeContactList 'ListName' {
  // variables with the % sign inherit defaults from control parameters
  // 1. Select lists
  EdgeList 'FirstEdgeListName'
  EdgeList 'SecondEdgeListName'
  // 2.
  Edge1Thickness 0.4 cm   // minimum radius for edges of list 1 {1} %
  Edge2Thickness 0.2 cm   // minimum radius for edges of list 2 {1} %
  // 3. Define detection distance
  DetectionDistance 0.6 cm  // {2} %
  // 4. Define update interval
  UpdateInterval 0.000010 s  // [6] discontinued Jun-2011
  MinimumDistance 0.1 cm
  // 5. Enter contact models {3}
  ContactForce PenaltyHyst { . . . }
  FrictionForce { . . . }
  RollingResistance { . . . }
  // 6. Other commands
  WritePlotFile {4}
  Debug 6
}
```

[1] The `Edge1Thickness` parameter is used to provide a minimum edge radius for calculating the gap between two edges. The distance 'dst' between two edges is defined as the shortest distance between any point on edge 1 and any point on edge 2. The 'gap' is defined as

```
gap = dst - R1 - R2
```

where `R1` is the radius of edge 1 and `R2` is the radius of edge 2. `R1` is the maximum of the actual edge radius `r1` and the edge thickness `T1`

```
R1 = max(r1, T1)
```

The edge radius `r1` is typically defined by the properties of edge list 1. Similar equations hold for `R2`. If the radii have been specified in the edge lists, the `Edge1/2Thickness` command can be omitted. At least one of the two lists must have a postive radius.

[2] The detection distance Dd for edge-edge contacts is used for selecting edge-edge pairs which are close enough that may come into contact. In this version, an edge-edge pair is selected when

```
dst = Dd + R1 + R2
```

using the definitions for 'dst', 'R1', and 'R2' from [1].

[4] The `WritePlotFile` command is used to generate a Quasar plot file that visualize the detected edge contacts at time 0. The plot contains only the edges that are used

in the contacts using the plot attributes (color and radii) defined in the respective edge lists. The files is named using the convention ecL-'listName'.plt.

[5] Contact forces are generated when the two edges penetrate each other. This occurs when the 'gap' becomes negative. To avoid contact forces at time 0, if the initial gap for a specific contact is negative, an offset value `g0` equal to the absolute value of the gap is applied for the rest of the simulation (obviously to that contact alone)

```
gap = dst - R1 - R2 + g0     g0 = max(-gap, 0) at time 0
```

[6] Update intervals are now specified in the `ControlParameters` section using the `GlobalUpdateTimeInterval` command.

16.3.1 Time History Commands

```
PlotList 'ListName' {
  . . .
  ecL-'ListName' NumberOfContacts
  ecL-'ListName' ActiveContacts
  ecL-'ListName' MinimumDistance
  ecL-'ListName' MinimumGap
  ecL-'ListName' NormalForce
  ecL-'ListName' X-Force
  ecL-'ListName' Y-Force
  ecL-'ListName' Z-Force
}
```

The difference between 'MaximumPenetration' and 'CurrentMaxPenetration'

16.4 Face Contact List

The face contact makes it possible to detect contacts between a list of nodes/particles and a list of triangular faces. For the purpose of contact, a node/particles takes a spherical shape and a triangular face takes a three dimensional smooth shape consisting of a thick plate surrouned by semi-cylindrical edges and spherical corners, reminding the shape of old Vicks cough drops. The spherical surfaces are centered at the three nodes defining the face. The radius of the edge cylinders and corner-spherical surfaces is half the thickness of the plate. The thickness of the plate is either provided by the face lists or defined via input. Contact between a node and a face begins when the exernal surfaces of the associated 3-D shapes start penetrating each other. It is possible that in some cases, a node can go through a face. Here are some scenarios:

- Nodes are small, faces are thin and the maximum contact force that can be generated ($F_{n,\max} = K(r_{node} + t_{face}/2)$ is not suffient for preventing crossing. Remedy: increase penalty stiffness.

- The relative velocity of the objects is so large and the time step so coarse, that the contact algorithm does not have a chance to work. Remedy: reduce time step to achieve accuracy.

Although it would be possible to insert logic in the code to detect these scenarios, the computational cost would be considerable. It make more sense for the user to be aware of these potentatial problems and take corrective actions when they occur.

The input commands for face contact list take the format

```
NodeFaceContactList 'Name' {
  // variables with the % sign inherit defaults from control parameters
  // 1.  Specify lists
  NodeList 'NodeListName'
  FaceList 'FaceListName'
  // 2.  Enter minimum face thickness if necessary
  FaceThickness 0.2 cm   // {1} %
  // 3.  Enter node radius control parameters if necessary
  NodeThickness 0.4 cm   // {2} %
  // if nodes are particles, node thickness is the
larger of thn and node radius
  // 5. For contact purposes, nodes cannot be larger
than MaxNodeRadius
  [ MaxNodeRadius 0.6 cm ]
  // 6. All nodes are assigned a contact radius FixedNodeRadius
        independently of their actual radius
  [ FixedNodeRadius 0.5 cm ]
  // if face list comes from shells, face thickness is
     the larger of thf and half shell thickness
  // 7. Do not initialize overlap
  [ ActualContactDistance ] {4}
  // 8. Define detection distance
  DetectionDistance 0.6 cm  // %
  // 9. Define update interval
  UpdateInterval 0.000010 s  // %
  MinimumDistance 0.1 cm
  // 10. Enter contact models, see previous sections
  ContactForce PenaltyHyst { . . . }
  FrictionForce { . . . }
  RollingResistance { . . . }
  UpdateInterval 0.000010 s  // %
  Debug 6
}
```

[2] The radii of the nodes are controlled by three optional input commands: `NodeRadiusNoSmallerThan`, `NodeRadiusNoLargerThan`, and `NodeRadiusExactly`. The first command sets a lower

bound $r_{\min}$ for the node radii, the second command sets un upper bound $r_{\max}$, and the third command sets both lower and upper bound essentially forcing all nodes to have that value. These bounds are usedin the calculation to compute the effective contact radius rc for each particle using this logic

```
rc = max(rad, r_min)
rc = min(rc, r_max)
```

[4] The `ActualContactDistance` command is used in rare occasions when the initial configuration is pre-stressed and initial contact forces are desired. In this case, the `g0` gap offset parameter is never set.

16.4.1 Time History Commands

The following line commands are intended to be used inside Time History lists to produce records of global list variables.

```
TimeHistoryList HIST {
  . . .
  tcL-'ListName' NumberOfContacts
  tcL-'ListName' ActiveContacts
  tcL-'ListName' MinimumDistance [1]
  tcL-'ListName' MinimumGap
  tcL-'ListName' NormalForce
  tcL-'ListName' X-Force
  tcL-'ListName' Y-Force
  tcL-'ListName' Z-Force
}
```

[1] The `MinimumDistance` time history is very useful for checking whether any node has crossed a suface. This is likely to happen if the distance becomes very very close to zero.

16.4.2 Visualization

For models of moderate size which employ contact lists, it is useful to visualize the elements that can potentially come into contact at time zero. Such visualization provides 1) a way to check that thicknesses of points, edges, and faces are prescribed correctly, and 2) a way to assess that the detection distance parameter is adequate.

The visualization methods which were available in interactive `examine` mode have been improved and made available also in 'input file' mode as new commands. These new features are available in MARS versions dated April 19, 2010 or later.

The `WritePlotFile` command is used to generate a Quasar plot file that visualizes node-face contacts detected at time zero. The plot contains only the faces and nodes that are used in the contacts using the plot attributes (color and radii) defined in their respective lists. The file is named using the convention `tcL-'listName'.plt`.

16.5 Rebar Contact List

The rebar contact list makes it possible to detect contacts between a list of nodes/particles and a list of beam elements. For the purpose of contact, a node/particles takes a spherical shape and a beam takes a three dimensional smooth shape already described in the edge-edge contact section. This type of contact can be used for some specific applications, such as the interaction of loose particles with rebars.

The input commands for face contact list take the format

```
RebarContactList 'ContactListName' {
  // variables with the % sign inherit defaults from control parameters
  // 1.  Specify lists
  NodeList 'NodeListName'
  BeamList 'BeamListName'
  // 2.  Control paricle and beam shapes
  NodeThickness 0.4 cm // OBSOLETE
  NodeRadiusNoSmallerThan 0.2 cm
  NodeRadiusNoLargerThan 0.4 cm
  NodeRadiusExactly 0.3 cm
  BeamThickness 0.2 cm // OBSOLETE
  BeamRadiusNoSmallerThan 0.2 cm
  BeamRadiusNoLargerThan 0.4 cm
  BeamRadiusExactly 0.3 cm
  NoHemiSphericalCaps
  // 3.  Set detection and update parameters
  DetectionDistance 0.6 cm // %
  UpdateInterval 0.000010 s // %
  // 4. Enter contact models, see previous sections
  ContactForce PenaltyHyst { . . . }
  FrictionForce { . . . }
  RollingResistance { . . . }
  Debug 6
}
```

The radii of the nodes are controlled by three optional input commands: 'NodeRadiusNoSmallerThan', 'NodeRadiusNoLargerThan', and 'NodeRadiusExactly'. The first command sets a lower bound $r_{\min}$ for the node radii, the second command sets un upper bound $r_{\max}$, and the third command sets both lower and upper bounds to the same value essentially forcing all nodes to have that value. These bounds are used for computing the effective contact radius rc of each particle using this logic

```
rc = max(rad, r_min)
rc = min(rc, r_max)
```

Default values are $r_{\min} = 0$, $r_{\max} = M_{BIG}$ (very large number). Obviously, `NodeRadiusNoSmallerThan` and `NodeRadiusNoLargerThan` should not be used when `NodeRadiusExactly` is used to avoid prescribing conflicting bounds.

Similarly, the radii of the beam cylinders are controlled by three optional input commands: `BeamRadiusNoSmallerThan`, `BeamRadiusNoLargerThan`, and `BeamRadiusExactly`. The same logic is applied to compute and effective contact radius for each beam. If the beam has already a circular shape, the beam list provides a defult radius which is related to the geometric properties of the cross-section: for solid rebars, it is the actual radius; for hollow tubes, it is the outside radius, etc.

The command `NoHemiSphericalCaps` is optional and is used to control the 3D shape of a beam to be a plain cylinder with no hemispherical surfaces attached at the ends.

16.5.1 Time History Commands

The following line commands are intended to be used inside Time History lists to produce records of global list variables.

```
TimeHistoryList 'ListName' {
  . . .
  rcL-'ContactListName' NumberOfContacts
  rcL-'ContactListName' ActiveContacts
  rcL-'ContactListName' MinimumDistance
  rcL-'ContactListName' MinimumGap
  rcL-'ContactListName' NormalForce
  rcL-'ContactListName' X-Force
  rcL-'ContactListName' Y-Force
  rcL-'ContactListName' Z-Force
}
```

17 Interference Check

This is a collection of methods designed to detect part overlapping or crossing of a part through a surface. Their main purpose is to ensure that contact conditions work properly. These methods do not affect the results of a computation and should be disabled when the user has gained confidence that there is no unwanted part penetration. penetration.

17.0.2 Node-Hex Overlap Check

This feature is designed to detect whether any node from a list are located inside any hex element form another list. The main purpose of this is to ensure that the contact algorithms is able to prevent contacting nodes from penetrating into a solid part.

```
Checks {
  NodeHexOverlapCheck NHOC {
    NodeList NODS
    HexList HEXS
    CheckTimeInterval 0.1 ms
    [ Disable ]
```

```
  }
}
```

Make the CheckTimeInterval smaller than the time step to perform the check at every check, although this frequency is most likely execessive.

17.0.3 Node-Tet Overlap Check

This feature is designed to detect whether any node from a list are located inside any tet element form another list. The main purpose of this is to ensure that the contact algorithms is able to prevent contacting nodes from penetrating into a solid part.

```
Checks {
  NodeTetOverlapCheck NTOC {
    NodeList NODS
    TetList TETS
    CheckTimeInterval 0.1 ms
    [ Disable ]
  }
}
```

Make the CheckTimeInterval smaller than the time step to perform the check at every check, although this frequency is most likely execessive.

17.0.4 Node-Hex Overlap Check

This feature is designed to detect whether any node from a list crosses any face from a triangular list. The main purpose of this is to ensure that the contact algorithms is able to prevent contacting nodes from crossing through a plate or shell part.

```
Checks {
  NodeFaceCrossingCheck 'CheckName' {
    NodeList 'ListName'
    TrianFaceList 'ListName'
    FaceContactList 'ListName'
    CheckTimeInterval 0.1 ms
    [ Disable ]
  }
}
```

Make the CheckTimeInterval smaller than the time step to perform the check at every check, although this frequency is most likely execessive.

18 Pre- and Post-Processing

18.1 Plot Lists

The input section for plot lists is typically located at the end of the input stream, before the MPI section and at the same level of the time history sections. Multiple plot lists can be defined. Each plot lists generates a sequence of plot files at specified time intervals. Currently, two plot formats are available: Quasar and Paraview. There are two ways for selecting plot format. The first way is to specify it inside the `PlotList` section:

```
PlotList 'listName' {
  Paraview
  . . .
}
// or
PlotList 'listName' {
  Quasar
  . . .
}
```

If either keyword is omitted, MARS automatically assumes the plot format is Quasar. Since July 17, 2011, a second way of specifying plot format is available:

```
PlotList 'listName' Paraview {
  . . .
}
// or
PlotList 'listName' Quasar {
  . . .
}
```

The typical plot list input features control commands and list specific commands. The first group includes four commands:

```
PlotList 'listName' 'plotType' {
  TimeInterval 0.1 ms   // also dt 0.1 ms [1]
  DeleteAllFiles        // in this family  ( PLOT.* ) [2]
  Counter 44            // reset file name counter to 44 [3]
  NextTime 0.344 ms     // reset next plot write time [3]
  . . .
}
```

[1] The `TimeInterval` command is used to specify the time interval used for creating the family of plot files. Since Jul 17, 2011, this command may be omitted and a default `TimeInterval` can be specified in the `PlottingDefault` subsection of the `ControlParameters` section. For `Quasar` files, different plot lists can use different time

intervals. For Paraview files, graphical components are saved in different plot lists; as such, the time interval must be the same and the default time interval command is a better way for specifying the time interval.

[2] The `DeleteAllFiles` command is used to remove all plot files previuosly generated. For `Quasar` plot lists, Mars executes the command `rm 'listName'.???`. For Paraview plot lists, Mars executes the system commands `rm 'listName'.*.vtu` and `rm 'listName.*.pvd`.

[3] These two commands, `Counter` and `NextTime`, are rarely used. They may be useful in restart operations.

The rest of the input specifies the list[s] to be plotted and specific plotting attributes. More details are available for each of the plottable lists in their sections. Below are some examples.

```
PlotList 'listName' Quasar {
  . . .
  All  // plot all plottable lists
}
PlotList 'listName' 'plotType' {
  . . .
  hxL-WALL {
     CountourPlot StateVariable 1
  }
}
```

18.1.1 Parallel processing with Paraview

The MARS plot generating procedures for Quasar and Paraview are very different. Quasar expects a single input file; as such, the contributions to each list from the various processes must be combined in MARS. Paraview can read and combine files generated from different processes. This eliminates the need to combine large data sets in rank zero process, which could lead to memory requirement problems. The Paraview files have the following name convention `'plotListName'.nnn.ppp.vtu`, where `nnn` is an integer represeting the sequential time frame and `ppp` is a three-digit integer representing the rank of the process that generated the file. In addition to these files, there is an additional file name `'plotListName'.pvd` that contains direction for Paraview on how to load and combine the previous files. This is one of the files that shows up in the Paraview Open window, and it is the one that should be selected.

18.2 Time History Lists

The input section for time history requests is typically located at the end of the input deck after all components of the model have been defined and initialized. The name of the time history list is used to create the name of the output file by appending '.th'. The input commands to the TimeHistoryList consist of the output time interval and a set of variables, one variable per line. The format for each variable is standardized, and obeys the following convention convention

```
v [de 'Description'] [S scl] [O ofs] [D]
```

where ob is the two-character tag for a list (this is found in the examples at the list level in the pages for the different lists), NAME is the name of the list. The first line of the three lines above refers to variables for the whole model, such as total kinetic energy, a list of available variables is given below. If the variable involves the whole list, use the obL format; if the variable involves an object of the list, use the ob format and select the object o using one of the following methods:

1. enter the index of the object, e.g. nd-NODS 45
2. find object closer to a point in space, e.g. nd-NODS cl 5. 7. 3.

In the commands above, v is used to select the variable within the list or object. Optional entries are the description, which will be displayed in plots and used for variable selection, the scale scl and offset ofs. Scale and offset are used to modify the output value according to the following expression

```
Voutput = scl * (Vcalc + ofs)
```

The D character automatically sets the offset to the opposite of the initial value of the variable. This is useful when plotting displacements in a Cartesian direction since the displacement is equal to the difference between current coordinate and initial coordinate:

```
nd-NODS 12 cx D = displacement of node 12 in x-direction.
```

The variables available for each list and the keyword to specify them, are described in the various list pages under a section called 'Time Histories' Histories'

```
HistoryList HIST {
  TimeInterval 0.1 ms // also dt 0.1 ms
  SkipFirstRecord // use this when values at time 0 look wrong
  // enter a list of scalar quantites
  //  Global quantities
  tmx  // X-Translational momentum
  tmy  // Y-Translational momentum
  tmz  // Z-Translational momentum
  rmx  // X-Rotational momentum
  rmy  // Y-Rotational momentum
  rmz  // Z-Rotational momentum
  ke   // Kinetic energy
  ie   // Internal energy
  iw   // Internal work
  ew   // External work
  eb   // Energy balance
  kex  // Kin Energy vx
```

```
  key  // Kin Energy vy
  kez  // Kin Energy vz
  TimeStep // {1}
  CpuTimePerStep // {2}
  CumulativeCpuTime // {3}
  //  List type quantities
  ndL-Nodes variable [ options ]
  //  Element type quantities
  nd-Nodes index variable [ options ]
  // In the two exemples above nd means NodeList
  // For specific list formats, check in the history section of the list help
  // The following options are available to all lists
  S s : scale output by s
  O o : offset output by o
  combined:  output = s * (value + o)
  default: s = 1.   o = 0.
  D:  take difference between current and initial values
  U length in : convert a length variable into inches
  Node: U modifies the scaling factor s by multiplying
        current scaling factor to conversion factor
  F %6.3f : uses a specific format (C convention)
       %6.3f = 6 fields with 3 decimal digits
       %10.3E = exponential notation, 3 decimals
  de "Description" : change description
}
```

[1] The time history of the time step provides useful information regarding the evolution of the stable time step during a simulation. This can help when in time certain problem may occur.

[2] The time history of the CPU time per step samples the time it takes per cycle at the print intervals. The CPU time per step is typically constant, except for the step when plots are generated or contact conditions are updated. Some spikes in the curve are to be expected. For MPI performance evaluations, one should use the prevalent value.

[3] The time history of the cumulative CPU time tells how much CPU time has elapsed from the beginning of the execution. It is useful to detect if a considerable amount of time is spent in performing special tasks. For example, if the detection distance in a contact list was set very large, the time required to update the contacts may show up as a visible step in the time history curve.

19 MPI Parallel Processing

The MPI parallelization of MARS is work in progress that begun in the spring of 2009. The MPI approach adopted in MARS takes advantage of the object oriented architecture of MARS itself. itself.

Before the advent of multi-core processors, the term CPU was used to identify and count individual processor units in a computer system. This term can still be used to describe a physical object that sits in your machine, but when discussing resource allocation for parallel computing the words "CPU" and "processor" are ambiguous, and are therefore best avoided.

For instance, documentations of cluster resource allocation schemes typically make reference to "processors" as meaning essentially a core (as in "each node has two sockets and each chip has two cores, which means that each node has four equivalent processors"). It would then be very confusing to say that this cluster has two dual-core processors on each node!

Instead, we have a hierarchy of three levels that we deal with: cores, sockets, and nodes.

Node..: also called "host", "computer", "machine". For our purposes, the most important definitions of a node is that a certain amount of memory (RAM) is physically allocated on each node. Nodes are typically separated by network connections, and each node has a unique network address (host name/IP number). Each node contains one or more sockets; the node is then labeled e.g. a "two-socket" or "four-socket" node.

Socket: refers to collection of cores with a direct pipe to memory. Note that this does not necessarily refer to a physical socket chip, but rather to the memory architecture of the machine, which will depend on the chip vendor specifications. Usually, however, the sockets resemble the old definition of a CPU (or single-core processor). Each socket contains one or more cores; the socket is then labeled e.g. a "dual-core" or "quad-core" socket. Each socket has its own L2 cache chip, which typically is shared among its cores.

Core..: refers to a single processing unit capable of performing computations. A core is the smallest unit of resource allocation. Each core has its own L1 cache chip.

There are two reasons for distributing the computation over several processors:

1. for handling large models which require extensive memory to run in core,

2. for reducing execution time.

In the first case, we need to distribute our computational model over a sufficient number of nodes so that each node can accomodated the memory requirements for its portion of the calculations. In the second case, we want to take advantage of the simultaneous solutions of different parts of the model, which reduces global execution time. time.

In MPI executions, the user requests access to a certain number of nodes, which are allocated by the system when they become available. The computational model is partitioned into as many parts as the number of cores available. This operation is called 'domain decomposition'. The objective of 'domain decomposition' is to split the model in regions. Each of these regions is assigned to an individual core. different core involves distributing objects over various processors. Currently, every processor has complete exposure to the entire geometry of the model. This is accomplished by using the inheritance properties of OOP. For example, an LDPM element which is one of the most memory intensive and computationally demanding element, requires almost 6 kilobytes of memory per tet element. However, the geometry of a tetrahedral is defined by 4 nodes

which require either 16 or 32 bytes depending whether we use 4-byte integers of 8-byte addresses for identifing the nodes. During the reading phase, each processor reads and stores all tetrahedral elements in 'TetSolidList'. During the initialization phase, each processor converts the tet elements under its 'jurisdiction' from geometrical elements to LDPM elements. elements.

19.1 Decomposition Schemes

Currently, MARS provides three schemes for performing domain decomposition:

1. Orthogonal Recursive Bisection (ORB)
2. Octree
3. METIS libraries

The ORB method has been used extensively and is the recommended method. The octree method is inferior to the ORB method. The METIS approach is in a development stage. More information on the three approaches is given below.

19.1.1 Orthogonal Recursive Bisection

The orthogonal recursive bisection method surrounds the domain by a parallelepipedal box. The box is first divided in the longest direction in two smaller boxes each containing the same number of objects. Each of the two boxes are split into two smaller boxes and so forth, until the desired number of boxes (domains) is generated. Some figure and a more extensive explanation are given at these two web sites:

`http://www.netlib.org/utk/lsi/pcwLSI/text/node253.html`

`http://ww2.cs.mu.oz.au/498/notes/node52.html`

Currently, the orthogonal recursive bisection ('Bisect') method is the preferred domain decomposition in Mars. The input commands for ORB are:

```
Bisect 'Label' {
  List ttL-'ListName' // (Req.)
  FirstNode 0   // [1]
  NodeSpan 128 // must be a power of 2  [1]
  Fixed // [2]
  [Verbose]
}
```

[1] If FirstNode and NodeSpan are not specified, MARS will use all available processors for the run. If NodeSpan is greater than the number of available processors, MARS will automatically reduce it.

WARNING: The keywords FirstNode and NodeSpan will be changed to FirstRank and RankSpan to reflect the common practise in MPI programming to refer the processes assigned to each core as 'rank 0', 'rank 1', etc.

[2] Without the `Fixed` option, the domain decomposition is updated as frequently as specified in the `GlobalUpdateTimeInterval` command in the `ControlParameter` section. When the domain decomposition is updated, lists are affected in different ways: nodes in node lists are redistributed, by default, elements are not migrated; active contacts are migrated across domains if necessary and new contacts are found within each domain.

In the next paragraphs, we will explain in detail how this parallelization scheme is implemented in MARS. The list selected by the user with the `List` keyword is used for the domain decomposition. As such, the user should select the most computationally expensive list in the model. In this case, computational cost is defined as the number of elements in the list times the computational cost of each element. The center points of the elements are then used to drive the ORB process and split the domain in a set of subdomains. Since the number of subdomains doubles at each step, the total number of subdomains is a power of two. For this reason, the number of core requested for an MPI run should also be a power of two number. If a different number of cores is requested, MARS will error off with a message. The ORB is extremely fast and a large number of points, in the order of millions, can be split in multiple subdomains in less than a second on most current processors.

Once the domain decomposition has been completed, the whole three-dimensional space is subdivided in finite or semi-infinite parallelepipedal regions. Each region is assigned to a single core. Thus, the number of regions has to be equal to the number of cores been requested. Although it is possible to specify `FirstNode` and `NodeSpan`, these features are temporarily disabled and MARS will perform the domain decomposition based on the number of cores available.

The domain decomposition is used to assign the objects of most lists to the cores. Some lists, like `PlotLists` and `TimeHistoryLists` are excluded from this process.

19.1.2 Octree

The octree method creates a box that envelops the model and splits the box in 8 smaller boxes, by subdividing the domain in all three directions in space. It is a classic method but the number of objects in each domain may vary. In this respect it may not generate a well balanced distribution of computational work. More on this method at:

`http://en.wikipedia.org/wiki/Octree`

The octree method has been implemented in MARS, but only partially tested. Because ORB is so much superior to the Octree methods, the Octree decomposition is not being supported.

19.1.3 METIS decomposition

METIS is a set of serial programs for partitioning graphs, partitioning finite element meshes, and producing fill reducing orderings for sparse matrices. The algorithms imple-

mented in METIS are based on the multilevel recursive-bisection, multilevel k-way, and multi-constraint partitioning schemes.

`http://glaros.dtc.umn.edu/gkhome/views/metis`

The METIS decomposition works well for large meshes where the connectivities do not change during the course of a simulations. When the model consists of multiple lists, contact conditions, special constraints, it is more complicated to use METIS for assigning the work among all the cores. In this respect, the ORB is easier to program and execute.

19.2 Treating lists

In this section, we discuss the MPI strategy for treating different lists. Basically, there are three types of lists:

- Lists type L1: currently, only `NodeList` belongs to this type. Each rank containts the full description of all objects in these lists. An object in one of these lists can only be 'owned' by a single rank, but can be 'shared' by multiple ranks. An object is shared by a non-owner rank, when it is used in the definition of other objects that are owned by that rank. For example, rank 7 owns a tetrahedral element; two of the four nodes used to the define the element are also owned by rank 7, but the other two nodes are owned by a different rank. The latter two nodes are marked as shared by rank 7.

- Lists type L2: most of finite element lists belong to this type. Each rank contains a full description of the objects it owns, and a reduced geometric description of all the other objects it does not own. This makes it possible to perform certain operations, like contact detection, by all ranks at any time.

- Lists type L3: variable lenght lists, like contact condition lists, belong to this tpye. Typically, the objects in these lists are created during the initialization phase. During the initialization phase, the objects are created only in the rank that controls the domain where the objects are located. located.

19.3 MPI Logic

This section explains the logic currently implemented for synchronizing the message passing between the processes. With reference to the 'solver loop' previously discussed, the operations for synchronising nodal information at the inter-domain boundaries are performed within the `integrateEOM` method.

```
while (time < terminationTime) {
    . . .
    for (jL = 0; jL < numLists; jL++)
        list[jL]->calcFrc();
    for (jL = (numList-1); jL > -1; jL--)
```

```
        list[jL]->reduceFrc();
    for (jL = 0; jL < numLists; jL++)
        list[jL]->integrateEOM();
    // apply kinematic conditions for master-slave formulations
    for (jL = 0; jL < numLists; jL++)
        list[jL]->applyKin();
    . . .
```

The treatment of the boundary nodes is explained with this example. Assume you have a finite element `Q` owned by the rank 1 process. Two of its nodes, 6 and 9, are also owned by rank 1 while nodes 7 and 8 are owned by rank 2. The internal forces for `Q` are computed in the `calcFrc()` method. The force contributions at node 7 and 8 are passed to rank 2 via an MPI message at the beginning of the `integrateEOM)()` method. These contributions are added to the existing forces. The equations of motion are then integrated. Finally, the updated coordinates and velocities for nodes 7 and 8 are passed back to rank 1, that will use them for the next time step.

```
Rank 1  | Rank 2
 6--------7
 |   Q  | |
 |      | |
 9--------8
```

This logic works very well for all types of list that compute internal forces, including contact conditions, penalty-force based constraints, etc.

The current logic is not able to handle master-slave constraints. This is explained with the following example. Let's consider a rebar embedded in a solid tetrahedral LDPM mesh. Let `B` be a beam element for the rebar that spans two domains, one owned by the rank 1 process and the other owned by the rank 2 process, as shown schematically below:

```
Rank 1  | Rank 2
--8----B---9--
        |
```

Beam `B` is owned by rank 1, its nodes, 8 and 9, are owned by rank 1 and rank 2 respectively. The internal forces computed for beam `B` at node 9 in the `calcFrc()` method must eventually be transferred to rank 2 that ownes node 9. Currently this is done in the `integrateEOM()` method. Assume that the beam nodes are embedded in a tetrahedral mesh using master-slave constraints. The force reduction where forces at beam nodes are distributed to tet nodes is done in the `reduceFrc()` method which is placed between the `calcFrc()` and `integrateEOM()` methods. With the current logic, node 9 has not yet received the force contribution from beam `B`.

Similar problems may occur when synchronizing the velocities. For this scenario, let's assume that the constraint that ties node 9 and a tet elements is owned by the rank 1 process. The information for the tet nodes is synchronized in the `integrateEOM()`. Thus, the velocities at the beam nodes are computed correctly. However, the velocities

for node 9 computed by rank 1 in the `applyKin()` method are not shared with the other processes. Indeed, after the `applyKin()` task, rank 1 should communicate the velocities of node 9 to rank 2 that is the owner of node 9 and rank 2 should communicate the same info to all other ranks that use node 9.

We are currently evaluating different strategies for including master-slave constraints in the overall MPI framework. Obviously, one of the requirements for any strategy is the minimization of the number of inter-process mpi messages.

19.4 Visualization

It is possible to visualize the domain decomposition for some lists. Currently this option is available for 1) node lists, and 2) tet lists. Details are given in the plot help sections of these lists.

```
PlotList DomainDecomposition {
  Paraview
  TimeInterval 100. s
  ttL Tile {
    DomainDecomposition 1.3
  }
}
```

19.5 Examples

19.5.1 Brazilian Test

The top and bottom plates and all contacts of plates with specimen are handled by rank 0. The rest of the model is split among all other processors using the ORB method.Slaves nodes in contact are also assigned to rank 0. 0.

```
MpiDomainList {
  SingleNode DD1 { Node 0 }
  Bisect DD2 { FirstNode 0 List ttL-Speciment Verbose }
  *-TopPlate DD1
  *-BottomPlate DD1
  *-Specimen DD2
  PrintDetails
}
```

19.5.2 Contact between projectile and concrete slab

LDPM elements are decomposed using ORB. The projectile which is relatively inexpensive is assigned to the rank 0 process. Fiber and conrcrete-fiber interaction constraints are distributed using the DD2 decomposition.

```
MpiDomainList {
  SingleNode DD1 { Node 0 }
  Bisect DD2 { FirstNode 0 NodeSpan 32  List ttL-Tile Verbose }
  Default DD1
  nd-Fibers DD2
  *-Tile DD2
  *-FSP DD1
  nc-FSPTile DD2
}
```

19.5.3 Contact between particles and nanoindenter

Particles are divided using recursive bisection method. Nanointenter is handled by all nodes. Contact between particles and nanoindenter are handled by RB. Contact between particles are handled by RB

```
MpiDomainList {
  SingleNode DD1 { Node 0 }
  Bisect DD2 { FirstNode 0 List ndL-Particles Verbose }
  AllNodes DD3
  Default DD1
  npL-PrtInteraction DD2 U
  nd-Particles DD2 U
  ndL-NanInd DD3 C
  tcL-PrtIndContacts DD2 U
  Update {
    TimeInterval 0.1 ms
    [ dd-DD2 ]
    nd-Particles
    nc-*
    tc-*
  }
}
```

20 Generation of Complex Parts

21 How to Perform Specific Tasks

This is a collection of instructions that describe procedures for performing various taks.

21.1 monitor energy

In most dynamic simulation, it is useful to monitor the transfer of energy across the system. Most important, it is essential to ensure that there is no artificial energy entering

into the system due to numerical instabilites or just errors in the algorithms. The best way to accomplish this control in MARS is to generate time histories of work and energy for global and list variables. At the global level, four quantities are available:

```
TimeHistoryList 'ListName' {
  . . .
  ExternalWork
  InternalWork
  KineticEnergy
  EnergyBalance
}
```

'ExternalWork' (We) is the work performed by external forces, or pressures, or reactions at nodes where the motion is prescribed. Positive external work means that the nodes move in the directions of the forces and energy is entering into the system.

'InternalWork' (Wi) is the work performed by internal stresses as a body is deforming. If the strains operate in the direction of the stresses (for example, tensile strain increments are applied to a body already in tension), then the internal work is positive. For nonlinear materials, internal work will result in recoverable elastic energy and dissipated energy (e.g. due to plastic work). An internal work quantity is computed for each list that consists of entities with internal forces (finite elements, contact elements, bonding elements, etc.). The computation of the internal work is done just before the node force increments are added to the total nodal force variable.

$$W_i += \sum F_{Ij}(t_i)V_{Ij}(t_i - dt/2)dt$$

where F_{Ij} are the force increments and V_{Ij} are the corresponding velocities. Note that the velocities are half a step off from the forces; this may result in small errors.

'KineticEnergy' (Ek) is the energy associated to the motion of the parts and is the summation of of

$$E_k = 1/2 \sum m_i v_i^2$$

where m_i and v_i are the masses and velocities of the nodes. The kinetic energy is always positive.

'EnergyBalance' Eb is defined as

$$E_b = W_i + K_e + W_e$$

The energy balance should remain constant during a calculation. If a system starts in its unstressed state but with moving parts, the intitial energy balance is the total kinetic energy of the moving parts at the beginning of the simulation.

It is possible to print a global table of external, internal, and kinetic energy per list like the one shown below when MARS is interactive mode, by typing 'M' and 'w' at the prompt:

```
mdl> M
n: number of elements
m: mpi decompositions
w: work balance
x: node lists
```

```
t: min time steps
> w
List              | ExtWrk | IntWrk | KinEnr
-------------------------------------------
nd-PRTC           |        |        |  0.119
tt-PRTC           |        | -0.736 |
nd-EFEP           |        |        |  0.006
hx-EFEP           |        | -0.083 |
nd-EFEN           |        |        |  0.006
hx-EFEN           |        | -0.076 |
nd-LOAP           |        |        |  0.059
hx-LOAP           |        | -0.013 |
pv-VEL1           |  1.098 |        |
tb-BND1           |        |  0.000 |
tb-BND2           |        |  0.000 |
-------------------------------------------
Totals            |  1.098 | -0.908 |  0.190
Balance = EW + IW - KE = -0.0004125
Work and energy values are times e-1 J
```

Example. This example, consisting of a spring 'SSSSS' fixed at the left and with a mass 'M' attached at the right (see schematic below), is intended to illustrate the concepts above in a simple framework.

```
|-SSSSSS-M  <- F
```

A constant force 'F' is applied at time t = 0. The closed form solution to this problem is is

```
x(t) = A (1 - cos wt)
v(t) = V sin wt
```

where w = sqrt(M/K) is the frequency, K is the stiffness of the spring, x(t) is the coordinate of the mass (x(t=0)=0.), A=F/K is the amplitude of the oscillations, v(t) is the velocity of the mass, V=A/w is the amplitude of the velocity. Thespring internal force Fi is computed as

$$F_i(t) = Kx(i) = AK(1 - \cos(\omega t) = F(1 - \cos(\omega t)$$

The external work We, internal work Wi, and kinetic energy become become

```
We(t) = F x(t) = F x(t) = F A (1 - cos wt)
      = F^2/K (1 - cos wt)
Wi(t) = integral [ Fi(t) v(t) dt ]
      = 0.5 K x(t)^2 =
      = 0.5 K A^2 (1 - cos wt)^2
      = 0.5 F^2/K (1 - 2 cos wt + cos^2 wt)
      = 0.5 F^2/K (-1 + cos^2 wt) + F^2/K (1 - cos wt)
```

```
          = - 0.5 F^2/K sin^2 wt + F^2/K (1 - cos wt)
    Ke(t) = 0.5 M v(t)^2 = 0.5 M V^2 sin^2 wt
          = 0.5 F^2/K sin^2 wt
since
    M V^2 = M A^2 / w^2 = M (F/K)^2 / (M/K) = F^2/K
```

Note that the external work is equal to the sum of internal work (in this case it is all in the form of elastic energy) and kinetic energy

$$W_e(t) = W_i(t) + K_e(t)$$

The energy balance Eb = Ke+Wi-We remains constant at 0.

21.2 save plot data for later post-processing

While MARS makes it possible to generate pre-determined plotting data through PlotLists during a simulation, you may find it necessary to change some of the plotting parameters once the results of a simulation are known. Rerunning a lengthy simulation with different plotting parameters is not only inconvenient but wasteful and time consuming. For this reason, in 2008, we introduced the capability of writing plot data at regular intervals during the simulation and reading the data back for generation of plot files viewable with Quasar or other 3-D viewers. This feature is not 100

```
Mars Input File
ControlParameters {
  . . .
  WritePlotDataFile data.plt Every 0.1 ms
}
. . .
```

In the command above, plottable data is written to file 'data.plt'. You can change this name to any name you want.

Postprocessing the data is also simple. The idea is to use the same input file used in the simulation for initializing the MARS model database. However, instead of running a simulation, MARS reads the data frames from the plot data file at the intervals at which they were saved and generates the 3-D plot files as specified in the PlotLists. You may modify the input file for generating new plot lists or change plotting parameters in existing ones. The command for instructing MARS to read data from the input file is ProcessPlotDataFile and is inserted at the very end of the input file

```
Mars Input File
ControlParameters {
}
. . .
PlotList Plot1 {
// update any parameter
}
// insert new PlotLists
```

```
PlotList Plot2 {
}
ProcessPlotDataFile data.plt
EOF
Updates
11-24-09: works for MPI runs
```

21.3 write and read restart files

Restart files fulfill two useful functions:

1. they make it possible to restart a job that was terminated for a variety of reasons.
2. they make it possible to interactively post-process the data in a different computer.

There are three ways to direct MARS on when to create restart files:

1. in the input file,
2. when an execution is interactive mode,
3. via external command file.

In the input file, file-restart commands are written inside the ControlParameters block. Three forms are available as shown in the example below. More than one line can be entered.

```
ControlParameters {
  . . .
  WriteRestartFile AtTime 10. ms
  WriteRestartFile AtStep 10000
  WriteRestartFile Every 0.1 ms
}
```

If you are running MARS in interactive mode, MARS goes interactive at the beginning and end of an execution. When in interactive mode, enter the character D at the prompt to generate a restart file. It is also possible to force a restart-file write during a batch execution. To do so, change to the working directory where input and output files reside.

```
cd work-dir
```

and enter the following at the prompt

```
echo D > stop
```

At every step, MARS check if file `stop` is present. It this file is present, MARS reads its contents. The character `D` in `stop` forces MARS to write a one-time restart file; after that, MARS deletes file stop so that it is not present at the next time step.

MARS restart file names have the following format: `mars.rst.xxxxxx` where `xxxxxx` is a 6-digit number which represents the time in the simulation when the file was created. Typically, the time is given in micro-seconds. For example, `mars.rst.001456` was created when the simulation had reached a time of 1.456 milli-seconds. The time in micro-seconds works for most simulations. However, in some cases, the time scale is much shorter or longer. For simulations at the nano-scale (simulations that employ the Nano unit system), the time is expressed in pico-seconds. For simulations that exceed a second, the number of digits may increase. For example, `mars.rst.2000000` represents a restart file written at 2 seconds.

Restarting an execution is relatively simple. At the prompt type

```
> mars mars.rst.000450
```

MARS will recognize the restart file, load the data-base and go in interactive mode.

In a batch file, enter the command

```
mars B mars.rst.000450 > output.dat
```

In the Mars launcher, grab and drag the `mars.rst.xxxxxx` file from the left column into the command line and then press the execute button.

Restart files are portable across computer systems. They are written in binary format. MARS automatically detects whether they are written in little-endian format and converts them if necessary.

It is possible to make changes to the database, including adding new components to the model. In this case, the syntax is

```
mars modification.mrs R mars.rst.000450
```

where file `modification.mrs` follows the rules of conventional MARS input files. An example will be provided in the future.

21.4 pre-process input files

Since Dec-2009, MARS supports the capability of preprocessing input files using the same syntax employed for C and C++ source code. A useful overall description of the C preprocessor can be found at at

http://en.wikipedia.org/wiki/C_preprocessor

Gnu.org provides a more comprehensive description of all capabilities of the preprocessor at at

`http://gcc.gnu.org/onlinedocs/cpp/index.html\#Top`

Of interest are the sections regarding conditional compilations. compilations.

The idea is to incorporate pre-processing directives in a MARS input file and use the preprocessing capabilites of the C compiler available on different platforms to generate the actual input file to be used as input to MARS. While the sites above provide a complete overview of the preprocessor capabilities, the examples below give a more tangible feel for how these capabilites can be used in the context of writing MARS input files. files.

The first example shows how to manage two executions with a single input file. The first execution performs the actual simulation and saves 'plot snapshots' at regular time interval of DT milliseconds. The second execution post-processes the plot data file generated in the first execution and generates a sequence of Paraview plot files. In addition, we want to be able to change the time interval at which plot snapshots and Paraview plot files are generated. The composite input file (input.mrs) looks like this: this:

```
Title line
ControlParameters {
  . . .
  WritePlotDataFile data.plt Every DT ms
}
#ifdef PLT
PlotList Cells {
  Paraview
  TimeInterval DT s
  ttL-Tile { Cells }
}
ProcessPlotData data.plt
#endif
EOF
```

where the preprocessing directives are the lines which begin with a '#' character. The C-preprocessor commands for generating the simulation input file 'inputS.mrs' are are

t[CC -E -DDT=0.001 input.mrs ¿ inputS.mrs]

where `CC` is the C/C++ compiler name which varies on different computer platforms. CC works on jade, g++ work on computers that have the gnu c++ compiler installed, etc. The resulting file (inputS.mrs) will look like this this

```
Title line
ControlParameters {
  . . .
  WritePlotDataFile data.plt Every 0.001 ms
}
. . .
EOF
```

Note that the string `DT` in the input file is replaced by the definition given in the command line by `-DDT`. The switch `-D` indicates that what follows, in this case `DT`, is a macro with

an assigned value of 0.001. If no value is assigned to the macro, then, the preprocessor automatically assigns a value of 0. The C-preprocessor commands for generating the post-processing input file `inputP.mrs` are are

```
  CC -E -DDT=0.001 -DPLT input.mrs > inputP.mrs
The resulting input file looks like this
Title line
ControlParameters {
  . . .
  WritePlotDataFile data.plt Every 0.001 ms
}
. . .
PlotList Cells {
  Paraview
  TimeInterval 0.001 s
  ttL-Tile { Cells }
}
ProcessPlotData data.plt
EOF
```

In the examples above, the time interval parameter DT could have been defined inside the file input.mrs using the `#define` directive directive

```
This is the title
#define DT 0.001
ControlParameters {
  . . .
  WritePlotDataFile data.plt Every DT ms
}
#ifdef PLT
PlotList Cells {
  Paraview
  TimeInterval DT s
  ttL-Tile { Cells }
}
ProcessPlotData data.plt
#endif
EOF
```

The second example is more complex but shows the potential benefits of using preprocessing directives. Let's assume you have a complex model and want to perform a parametric study of a projectile impacting a structure at different speeds. Some of the problem parameters would change depending on the projectile speed. For example, for faster speed you may want to perform contact updates more frequently as well as plot dumps, while reducing the overall simulation time. This would require the creation of

multiple input files for each speed case. Furthermore, if the model needs to be modified, the modifications have to be applied to all files. This is a case where the conditional capabilities of the preprocessor come handy. Look at the input file below below

```
Title line
#if V0 == 100
  #define TEND  2.
  #define DT 0.02
#elif V0 == 200
  #define TEND  1.
  #define DT 0.01
#else
  #error "Velocity not accepted"
#endif
ControlParameters {
  . . .
  TerminationTime   TEND ms
  WritePlotDataFile data.plt Every DT ms
}
. . .
NodeList {
   . . .
   Set vz const V0 m/s
}
#ifdef PLT
PlotList Cells {
  Paraview
  TimeInterval DT s
  ttL-Tile { Cells }
}
ProcessPlotData data.plt
#endif
EOF
```

The mars input files for the two speed cases can be generated using the commands

```
CC -DV0=100 input.mrs > input2.mrs
```

or

```
CC -DV0=200 input.mrs > input2.mrs
```

21.5 import Ingrid meshes

The INGRID program can be used to generate finite element meshes of the complete model or parts of the model. Very often it is preferable to mesh individual components

separately and combine them later in the MARS input file. In these cases, the interaction between components, such as bonding or contact, can be defined very conveniently in the MARS input. INGRID generates an output file named ingrido, unless the user selects a different filename. MARS can read the ingrido file and convert its data to MARS format. This can be done in two ways.

The first method is the most recent and probably the most convenient because all steps are documented in input files.

• generate an input file that reads ingrido and saves the mesh into a MARS mesh file, for example

```
Ingrid conversion input
//------------------------------
ControlParameters {
  Units English
}
//------------------------------
Read Dyna3dInputFile ingrido
//------------------------------
NodeList NODS {
  Rename BLLT
}
//------------------------------
HexSolidList H000 {
  Rename BLLT
  Write PartMeshDataFile bullet.mrs
}
```

• the mesh can be easily imported into a MARS input file using the commands

```
HexSolidList BLLT {
  Material STEL
  Read bullet.mrs
}
```

The second method is more interactive but requires repetitive work each time a change in the mesh is necessary.

```
run  mars++ -D ingrido
```

At the interactive prompt you can examine the INGRID generated model as if it were a MARS model

When you are ready to write out the model in MARS format, return to the main level (-mdl- prompt) and type the W character

Select the mars output and this will generate a file name mars.out which contains the ingrido data converted to MARS format.

The mars.out file should be renamed to something more descriptive and should be edited so that the names of the lists are meaningful and unique.

Note. INGRID should be used mostly as a mesh generator. Some of the features in INGRID are not translated into MARS. For example, contact conditions specified in INGRID are not translated because MARS deals with contact at the list level (nodes from list A contacting faces from list B) and not at the object level (nodes, faces). Here is a partial list (to be complete) of features that are supported:

- node boundary conditions,
- solid elements
- shell elements
- beam elements
- load curves
- pressure faces

The aspect ratio of Ingrid meshes can be improved by moving the internal nodes. The example in Figure a) at the website page

`http://www.es3inc.com/mechanics/MARS/Online/HowTo.htm#_How_to_convert`

shows the mesh of a bullet generated using Ingrid. Note that the aspect ratio of some element (2 elements deep from the surface) can be improved by slightly moving the nodes. This is done in MARS by using the Smooth command after the mesh has been imported and before it is saved. The improved mesh after a series of 6 smooth commands is shown in Figure b).

```
HexSolidList H000 {
  Rename BLLT
  Smooth
  Smooth
  . . .
  Write PartMeshDataFile bullet.mrs
}
```

In the smoothing operations above, the displacements of the surface nodes are constrained to ensure that the external shape does not change. Thi is done by using nodal boundary conditions. The Ingrid input for the model above is listed below. Note how boundary conditions are used to fix the external nodes. Nodes at the bottom face are free to move in the bottom plane. Nodes on the plane of symmetry are free to move within the plane of symmetry. The boundary conditions need to be modified for the actual simulation.

```
Bullet
dn3d
mat 1 3
  ro 0.00025 e 10e6 pr 0.3
  endmat
start
  1 3 5 ; 1 3 5 7 9 ; 1 7 9 11 ;
```

```
  -1. -1. 0.
  -1. -1. 0. 1. 1.
  0. 5. 6. 6.
  di 1 2 ; 1 2 0 4 5 ; ;
  di 1 2 ; ; 3 4 ;
  di ; 1 2 0 4 5 ; 3 4 ;
  sfi ; -1 -5 ; 1 2 ; cy 0. 0. 0. 0. 0. 1. 2.
  sfi -1 ; ; 1 2 ; cy 0. 0. 0. 0. 0. 1. 2.
  sfi -1 ; ; 2 3 ; sp 0. 0. 5. 2.
  sfi ; -1 -5 ; 2 3 ; sp 0. 0. 5. 2.
  sfi ; ; -4 ; sp 0. 0. 5. 2.
  b  0 0 1  0 0 1  001000
  b  3 0 0  3 0 0  100000
  b  0 0 4  0 0 4  111000
  b  1 1 0  1 5 0  111000
  b  1 1 0  3 1 0  111000
  b  1 5 0  3 5 0  111000
  end
end
t 0.1
cont
}
```

21.6 add and remove list during a simulation

During the course of a simulation, it may be required to add or remove lists. For example, we may need to prestress a structure and then add a dynamic load when the structure has reached a state of quasi-equilibrium under the static loads. Or we may want to remove a component that is no longer necessary in the simulation and continue the calculations for the component of interest. This is possible using this approach. We can use the `Read` command inside the `ControlParameter` section to schedule reading of an input file at a certain time (see section ... in this manual). Inside this file, we can insert the commands.

```
ControlParameters {
  . . .
  Read removeBullet.mrs atTime 0.2 ms
```

The listing of file `removeBullet.mrs` may look like this

```
File removeBullet.mrs
Lists {
  Remove HexSolidList Bullet
  Remove NodeList Bullet
  Remove NodeNodeContactList BulletTile
}
EOF
```

The list type (e.g. `HexSolidList`) employ the same keywords that were used to create the list. Be carefull to remove all lists that reference directly or indirectly on the lists removed.

21.7 create custom versions of mars

Since Jan 2011, MARS supports the capability of creating custom versions of the code which incorporate user defined lists and/or user defined material models. In May 2011, we added two methods for supporting restart procedures. A user can write his/her own classes in a single file, for convenience we will name it `user.cpp`. Some examples are provided. Some knowledge of the C++ language is required.

The user interface is very flexible and makes it possible to define multiple lists and multiple materials simultaneously. The interface consists of two methods:

```
obLst *Model::createUserDefinedList (string, Reader *);
obLst *Model::readRstUserDefinedList (RstReader *, string);
Obj *Model::createUserDefinedObject (string, Reader *);
Obj *Model::readRstUserDefinedObject (RstReader *, string);
```

The functionality of the user defined lists and objects is achieved through the polymorphic properties inherited from the parent classes. *This will be explained better in future versions of the manual*

The basic user.cpp file with no definitions is listed below:

```
#include "mars.h"
// createUserDefinedList(...) and readRstUserDefineList(...)
// must always be defined
obLst *Model::createUserDefinedList (string nam, Reader *rdr) {
    rdr->error("No user list has been defined");
    return NULL;
}
obLst *Model::readRstUserDefinedList (RstReader *rst, string nam) {
    return NULL;
}
// createUserDefinedObject(...) and readRstUserDefinedObject(...)
// must always be defined
Obj *Model::createUserDefinedObject (string nam, Reader *rdr) {
    rdr->error("No user object has been defined");
    return NULL;
}
Obj *Model::readRstUserDefinedObject (RstReader *rst, string nam) {
    return NULL;
}
```

Currently, only Unix type platforms are supported. The modified executable is generated using a Makefile of this type:

```
CMP = system dependent compiler
COP = compiler dependent options
LNK = system dependend linker
LOP = linker dependent options
HDR = folder where mars.h is located
LIB = folder where libmars.a is located

marsU: user.o $(LIB)/libmars.a
          $(LNK) $(OPT) -o marsU user.o -L$(LIB) -lm -lz -lmars

user.o: user.cpp
          $(CMP) -I$(HDR) $(COP) -o user.o user.cpp
```

For example, ...

Note that the compiler has to be able to find the header file mars.h. This can be accomplished using the `-I$(HDR)` option in the compile line.

21.7.1 User defined list

As described in other sections of this documentation package, lists are used for implementing collections of homogenous objects, such as finite elements, contact elements, constraint elements, etc. This subsection is designed to help users create their own elements and lists that operate on them. Complete documentation on this subject would require extensive information. At this time we are providing a basic explanation with some examples. This documentation will be expanded in the future.

First, some knowledge of Object Oriented Architecture and Programming is required. Users who are not familiar with Object Oriented Programming concepts are encouraged to google words like 'c++ classes', 'c++ inheritance', 'c++ polymorphism', etc. These terms are used here assuming the reader has some understanding of their meaning.

We will describe the process using an actual example. In this demonstrative case, we will implement a 10-node Cosserat tetrahedral element with 42 degrees of freedom: 10x3 translational DoF's (for the 10 nodes) and 4x3 rotational DoF's (for the 4 vertex nodes). The class `CosseratTet10` is derived from the basic class `Tet` whose definition can be found in file `mars.h`. Addtional members are added: references to 6 mid-edge nodes, state variable arrays, etc. The definition for the new class is given below:

```
class TetCosserat10: public Tet {
  protected:
    Node *nM[6];
  public:
    TetCosserat10() { };
    virtual ~TetCosserat10() { };
    virtual void whatAmI() { cout << "10 node " << endl; };
    void setMidEdgeNodes(Node *n[6]) {
        for (int i=0; i<6; i++) nM[i] = n[i]; };
```

```
    void read(Reader *, Node **);
    real calcForces(Node **, real *, Node **, real *);
};
```

The list class that handles a collection of the new tet elements is named `ttL_Cosserat10` and is derived from the base class `ttLst` that handles the basic 4-node tetrahedral geometric element. By doing that, the new class inherits all the methods from the parent class, including mesh generation methods, post-processing methods, etc. Only a few polymorphic methods need to be written for the new class. The definition of the new list class is given below:

```
ass ttL_Cosserat10 : public ttLst {
  public:
    ttL_Cosserat10() : ttLst() { };
    ttL_Cosserat10(string nm) : ttLst(nm) { initList(); };
    virtual ~ttL_Cosserat10() { };
    void initList() { ttLst::initList(); };
    string getListSubType() { return "Cosserat10"; };
    Object *createNewObject() { return (Object *)(new Tet10()); };
    Tet *createNewTet() { return (Tet *)(new Tet10()); };
    bool processCommand(Reader *, string);
    void readLst(Reader *);  // polymorphic
    void initialize();  // polymorphic
    real calcFrc();  // polymorphic
    void insertMidEdgeNodes(); // list specific
    void examine();  // polymorphic
};
```

There are a few significant methods that need to be written. The first method, `void readLst(Reader *)`, is a polymorphic method invoked during the reading phase. This method reads the input file and interprets commands specific to the new list, either for entering parameters or for performing tasks:

```
void ttL_Cosserat10::readLst (Reader *rdr) {
    rd1 = rdr;
    while (true) {
        rdr->readLine();
        string lbl = rdr->getShortLabel();
        if (lbl == "}") {
            break;
        } else if (obLst::processCommand(rdr, lbl)) {
            if (rd2 == NULL) rdr = rd1; else rdr = rd2;
        } else if (ttLst::processCommand(rdr, lbl)) {
        } else if (processCommand(rdr, lbl)) {
        } else
```

```
            rdr->error("  Invalid keyword in tXLst::readLst");
    }
}
```

The second method, `void initialize()`, is also polymorphic and is invoked during the initialization phase. The purpose of this method is to initialize all elements.

```
void ttL_Cosserat10::initialize () {
    setStaticVariables();
    TetCosserat10 **tt = (TetCosserat10 **)ob;
    for (int i=0; i<num; i++)
        tt[i]->init();
}
```

The third method, `real calcFrc()`, is a polymorphic method invoked in the solver loop. The purpose of this method is to compute internal nodal forces withing each element based on its deformation history and deformation rate. This method looks like this.

```
real ttL_Cosserat10::calcFrc () {
    if (listIsNotActive()) return M_BIG;
    obLst::calcFrcInit(); // prints debug info if necessary
    setStaticVariables(); // set element static variable
    // setComputeTimeStep to true if element computes stable time step
    obLst::setComputeTimeStepFlag(false);
    // creates arrays for storing node pointers and relative force
    // and moment increments
    obLst::createArrays(10, 4);
    // the first argument, 10, is the number of nodes for which forces
    //      are computed, nodes per element with 3 translational DoF's
    // the second argument, 4, is the number of nodes for which moments
    //      are computed, nodes per element with 3 rotational DoF's
    Node **ndF = (Node **)obF;  // cast object pointers to node pointers
    Node **ndM = (Node **)obM;
    // cast object pointer to element pointers
    TetCosserat10 **tt = (TetCosserat10 **)lo;
    int i, ntt = nlo;
#ifdef _OPENMP
#pragma omp parallel private(i)
#pragma omp for
#endif
    for (i=0; i<ntt; i++)
        tt[i]->calcForces(ndF+10*i, f+30*i, ndM+4*i, m+12*i);
    // element forces and forces at the nodes are added to the nodes
    // in method procForces
    obLst::procForces();
    return M_BIG;
}
```

Note that if the element formulation had only translational Dof's, the method could be simplified to

```
    obLst::createArrays(10, 0);
    Node **ndF = (Node **)obF;
    TetCosserat10 **tt = (TetCosserat10 **)lo;
    int i, ntt = nlo;
    for (i=0; i<ntt; i++)
        tt[i]->calcForces(ndF+10*i, f+30*i);
```

The force and moment increments are saved in arrays `f` and `m` and later added to the nodes in method `procForces()`. This is done to avoid memory overwriting within the OpenMP parallel loop containing the calcForces element method.

In addition to the three polymorphic methods discussed above, there are two methods that are relevant. The first method `bool processCommand(Reader *, string)` is used to process list specific input commands, such as `InsertMidEdgeNodes` and loooks like this:

```
bool ttL_Cosserat10::processCommand (Reader *rdr, string lbl) {
    if (lbl == "InsertMidEdgeNodes") {
        insertMidEdgeNodes();
    } else
        return false;
    return true;
}
```

The second method is `void insertMidEdgeNodes()` and like the name says, its purpose is to add mid-edge nodes to a regular 4-node tetrahedral mesh and convert it to a 10-node tratrahedral mesh.

The element formulation is implemented in method `TetCosserat10::calcForces()`. The example below shows how to retrieve the current element data and how to save the computed forces and moments at the nodes in the global list array for later processing.

```
real TetCosserat10::calcForces (Node **ndF, real *f, Node **ndM, real *m) {
    // retrieve nodal coordinates and velocties
    real c0x = nd[0]->getCx();  // coordinate, node 0, direction x
    real v0x = nd[0]->getVx();  // velocity, node 0, direction x
    real w0x = nd[0]->getwx();  // rotation rates, node 0, direction x
    . . .
    // enter detail of formulation here
    . . .
    // store nodes and forces in arrays
    ndF[0] = nd[0];  // vertex nodes (force array)
    ...
    ndF[4] = nM[0];  // midnodes (force array)
    ndM[0] = nd[0];  // vertex nodes (moment array)
```

```
    f[ 0] = f0x;  f[ 1] = f0y;  f[ 2] = f0z;  // forces at node 0
    f[ 3] = f1x;  f[ 4] = f1y;  f[ 5] = f1z;  // forces at node 1
    . . .
    m[ 0] = m0x;  m[ 1] = m0y;  m[ 2] = m0z;  // moments at node 0
    . . .
    return M_BIG;
}
```

21.7.2 User defined material

In the MARS architecture, the class `Material` is derived from the generic class `Obj`, which includes various types of entities, such as `ReferenceSystem's`, `LoadCurve's`, etc. The new material is integrated in the Mars architecture using the `Model::readUserDefinedObject()`.

```
class myMaterial : public Material {
  . . .
}
  . . .
Obj *Model::createUserDefinedObject (string nam, Reader *rdr) {
    return new myMaterial(nam);
}
```

The class definition for a new material follows the pattern below (the class name `myMaterial` can be replaced by any other name which is not already used for defining another class. In the name has already been used, this will be apparent during compilation.

```
class myMaterial : public Material {
  private:
    // parameters for material model
  public:
    myMaterial() { };
    myMaterial(string n) : Material(n) { };
    ~myMaterial() { };
    void read(Reader *);
    // other methods
```

The best way to write a new material model is to start from an existing model; for example, the linear elastic material model which is made available by request and includes comments. There are several polymorphic methods, which may need to be defined depending on the model formulation and required functionality. This is also described in the sample section.

In the input file, the new material is defined using the command `UserDefinedObject` and later refereced as any other material.

```
UserDefinedObject Steel {
  // input data
```

```
}
HexSolidList Part FBSingleIP {
  Material Steel
  . . .
```

21.7.3 User defined mesh generator

Below is an example of an `Obj` class whose only purpose is generating a mesh by taking advantage of the Mars methods.

```
#include "mars.h"

class GenCube : public Obj {
  public:
    GenCube(string nam) : Obj(nam) { };
    ~GenCube() { };
    void read(Reader *);
};

void GenCube::read (Reader *rdr) {
    real edge = 0.; // length of edge
    int nel = 0;    // number of elements per side
    while (true) {
        string lbl = rdr->getShortLabel();
        if (lbl == "{") {
        } else if (lbl == "}")
            break;
        else if (lbl == )
            rdr->readLine();
        else if (lbl == "Side")
            edge = rdr->readLength();
        else if (lbl == "Elements")
            nel = rdr->getInt();
        else
            rdr->error("Invalid keyword in GenCube::read");
    }
    int i, j, k;
    int nps = nel + 1;
    int nnd = nps * nps * nps;
    ndLst *ndL = new ndLst("Cube");
    ndL->allocate(nnd);
    real crx, cry, crz, dc = edge/nel;
    // generate nodes
    Node ****nd = new Node***[nps];
    for (i=0; i<nps; i++) {
```

```
        nd[i] = new Node**[nps];
        crx = i * dc;
        for (j=0; j<nps; j++) {
            nd[i][j] = new Node*[nps];
            cry = j * dc;
            for (k=0; k<nps; k++) {
                crz = k * dc;
                nd[i][j][k] = new Node(crx, cry, crz);
                ndL->append(nd[i][j][k]);
            }
        }
    }
    hxLst *hxL = new hxLst("Cube");
    hxL->setNodeList(ndL);
    int nhx = nel * nel * nel;
    hxL->allocate(nhx);
    Node *n1, *n2, *n3, *n4, *n5, *n6, *n7, *n8;
    Hex *hx;
    // generate hex solid elements
    for (i=0; i<nel; i++) {
        for (j=0; j<nel; j++) {
            for (k=0; k<nel; k++) {
                n1 = nd[  i][  j][  k];
                n2 = nd[i+1][  j][  k];
                n3 = nd[i+1][j+1][  k];
                n4 = nd[  i][j+1][  k];
                n5 = nd[  i][  j][k+1];
                n6 = nd[i+1][  j][k+1];
                n7 = nd[i+1][j+1][k+1];
                n8 = nd[  i][j+1][k+1];
                hx = new Hex();
                hx->setNodes(n1, n2, n3, n4, n5, n6, n7, n8);
                hxL->append(hx);
            }
        }
    }
    ndL->reindex();
    hxL->reindex();
    Lists *lists = (Lists *)lst;
    // add list to general
    lists->addLst(ndL);
    lists->addLst(hxL);
}

// --------------------------------------------------------------------
```

```
// createUserDefinedList(string) must always be defined

obLst *Model::createUserDefinedList (string nam, Reader *) {
    return NULL;
}

// ----------------------------------------------------------------------
// createUserDefinedObject(string) must always be defined

Obj *Model::createUserDefinedObject (string nam, Reader *) {
    return new GenCube(nam);
}
```

A sample input for generating a 2. in cube with 5 elements per side is given below:

```
Generation of hex element cube
ControlParameters {
  Units English
}
UserDefinedObject Cube {
  Side 2. in
  Elements 5
}
EOF
```

21.7.4 User defined load curve

Below is an example of an `Obj` class derived from the `LoadCurve` class that implements a sinusoidal force function:

```
#include "mars.h"
// ----------------------------------------------------------------------
class SinFunction : public LoadCurve {
  private:
    real A;   // amplitude
    real w;   // frequency
  public:
    SinFunction(string nam) : LoadCurve(nam) { };
    ~SinFunction() { };
    void read(Reader *);
    real interp(real x) { return (A*sin(w*x)); };
};
void SinFunction::read (Reader *rdr) {
    A = w = 0.;
    while (true) {
        string lbl = rdr->getShortLabel();
```

```
        if (lbl == "{") {
        } else if (lbl == "}")
            break;
        else if (lbl == "")
            rdr->readLine();
        else if (lbl == "Frequency")
            w = rdr->readFrequency();
        else if (lbl == "Amplitude")
            A = rdr->readForce();
        else
            rdr->error("Invalid keyword in SinFunction::read");
    }
}
// ------------------------------------------------------------------
// createUserDefinedList(string) must always be defined
obLst *Model::createUserDefinedList (string nam, Reader *) {
    return NULL;
}
// ------------------------------------------------------------------
// createUserDefinedMaterial(string) must always be defined
Obj *Model::createUserDefinedObject (string nam, Reader *) {
    return new SinFunction(nam);
}
```

21.7.5 Multiple lists and objects in a single user.cpp file

Because the `SinFunction` is derived from the `LoadCurve` function, it can be referenced by its name in every class that employs a load curve for specifying a relationship. For example, the load function above can be used for specifying nodal loads.The versatility of the user-defined interface makes it possible to introduce any number of different lists and objects simultaneously. This is accomplished as shown in the example below:

```
#include "mars.h"
// ------------------------------------------------------------------
class MyFirstTetList : public ttLst {  // user defined tet list
    . . .
}
// ------------------------------------------------------------------
class MySecondTetList : public ttLst { // another user defined tet list
    . . .
}
// ------------------------------------------------------------------
class MyHexList : public hxLst {  // user defined hex list
    . . .
}
```

```
// ------------------------------------------------------------------
class MyMaterial : public Material { // user defined material
    . . .
}
// ------------------------------------------------------------------
class MyLoadCurve : public LoadCurve { // user define load curve
    . . .
}
// ------------------------------------------------------------------
// createUserDefinedList(string) must always be defined
obLst *Model::createUserDefinedList (string nam, Reader *rdr) {
    string lbl = rdr->getShortLabel();
    if (lbl == "MyFirstTetList")
        return new MyFirstTetList(nam);
    else if (lbl == "MySecondTetList")
        return new MySecondTetList(nam);
    else if (lbl == "MyHexListList")
        return new MyHexList(nam);
    rdr->error("Invalid keyword for user defined list type");
    return NULL;
}
// ------------------------------------------------------------------
// createUserDefinedMaterial(string) must always be defined
Obj *Model::createUserDefinedObject (string nam, Reader *) {
    string lbl = rdr->getShortLabel();
    if (lbl == "MyMaterial")
        return new MyMaterial(nam);
    else if (lbl == "MyLoadCurve")
        return new MyLoadCurve(nam);
    rdr->error("Invalid keyword for user defined object type");
    return NULL;
}
```

These classes would be accessed in the input file using the following isntructions:

```
UserDefinedList 'materialName' MyMaterial {
  . . .
}
UserDefinedList 'curveName' MyLoadCurve {
  . . .
}
UserDefinedList 'listName' MySecondTetList {
  Material 'materialName'
  . . .
}
```

Note that it is not necessary to put all the coding in a single user.cpp file. Indeed, it is possible to create multiple files for improved readability. The above example could be arranged as follows:

Header file for class MyFirstTetList

```
class MyFirstTetList : public ttLst {
    . . .
};
```

Source file for class MyFirstTetList

```
#include "mars.h"
#include "MyFirstTetList.h"
void MyFirstTetList::method1 {
    . . .
}
. . .
```

Header file for class MySecondTetList

```
class MySecondTetList : public ttLst {
    . . .
};
```

Source file for class MySecondTetList

```
#include "mars.h"
#include "MySecondTetList.h"
void MySecondTetList::method1 {
    . . .
}
. . .
```

Header file for class MyHexList

```
class MyHexList : public hxLst {
    . . .
};
```

Source file for class MyHexList

```
#include "mars.h"
#include "MyHexList.h"
void MyHexList::method1 {
    . . .
```

```
}
. . .
```

Header file for class MyMaterial

```
class MyMaterialList : public Material{
    . . .
};
Source file for class MyMaterial
#include "mars.h"
#include "MyMaterial.h"
void MyMaterial::method1 {
    . . .
}
. . .
```

Source file for user.cpp

```
Source file for user.cpp
#include "mars.h"
#include "MyFirstTetList.h"
#include "MySecondTetList.h"
#include "MyHexList.h"
#include "MyMaterial.h"
#include "MyLoadCurve.h"
// createUserDefinedList(string) must always be defined
obLst *Model::createUserDefinedList (string nam, Reader *rdr) {
    string lbl = rdr->getShortLabel();
    if (lbl == "MyFirstTetList")
        return new MyFirstTetList(nam);
    else if (lbl == "MySecondTetList")
        return new MySecondTetList(nam);
    else if (lbl == "MyHexListList")
        return new MyHexList(nam);
    rdr->error("Invalid keyword for user defined list type");
    return NULL;
}
// createUserDefinedMaterial(string) must always be defined
Obj *Model::createUserDefinedObject (string nam, Reader *) {
    string lbl = rdr->getShortLabel();
    if (lbl == "MyMaterial")
        return new MyMaterial(nam);
    else if (lbl == "MyLoadCurve")
        return new MyLoadCurve(nam);
```

```
    rdr->error("Invalid keyword for user defined object type");
    return NULL;
}
```

Make file

```
Make file

OBJ = user.o MyFirstTetList.o MySec

marsU: $(LIB)/libmars.a $(OBJ)
        $(LNK) -o marsU -L$(LIB) $(OPT) $(OBJ) -lm -lz -lmars

MyFirstTetList.o: MyFirstTetList.cpp MyFirstTetList.h $(INC)/mars.h
        $(CMP) $(OPT) MyFirstTetList.cpp $<

MyFirstTetList.o: MyFirstTetList.cpp MyFirstTetList.h $(INC)/mars.h
        $(CMP) $(OPT) MyFirstTetList.cpp $<

MyHexList.o: MyHexList.cpp MyHexList.h $(INC)/mars.h
        $(CMP) $(OPT) MyHexList.cpp $<

MyMaterial.o: MyMaterial.cpp MyMaterial.h $(INC)/mars.h
        $(CMP) $(OPT) MyMaterial.cpp $<

MyLoadCurve.o: MyLoadCurve.cpp MyLoadCurve.h $(INC)/mars.h
        $(CMP) $(OPT) MyLoadCurve.cpp $<

MyMaterial.o: MyMaterial.cpp MyMaterial.h $(INC)/mars.h
        $(CMP) $(OPT) MyMaterial.cpp $<
```

21.7.6 Restart Procedures

If user defined objects or lists must be able to accomodate restart procedures, additional methods must be defined

```
string getTag();
void writeRst(RstWriter *);
void readRst(RstReader *);
Obj *Model::readRstUserDefinedObject(...);
obLst *Model::readRstUserDefinedList(...);
```

The method `getTag()` must return the string `"uO"` for user defined objects and `"ud"` for user defined lists. This strings are written to the restart file and used during restart to redirect the instantiation of object or lists to the `readRstUserDefinedObject()` and

`readRstUserDefinedList()` respectively. If a single object or list are defined, then these two methods are trivial:

```
Obj *Model::readRstUserDefinedObject (RstReader *rst, string nam) {
    return (new myNewObject(nam))
}
obLst *Model::readRstUserDefinedList (RstReader *rst, string nam) {
    return (new myNewList(nam))
}
```

If multiple objects or lists are defined in user.cpp, then the readRst methods must be able to instantiate the proper object or list. This can be accomplished using the names of the objects or lists, for example:

```
Obj *Model::readRstUserDefinedObject (RstReader *rst, string nam) {
    if (nam == "LoadHist")
        return (new myLoadCurve(nam))
    else if (nam == "Steel")
        return (new myMaterial(nam))
}
```

Using object/list names makes the method above dependent on the input file. If it is necessary to make the processure input file independent, ES3 will help you write the proper coding.

The methods `writeRst()` and `readRst()` are used to save the data to the restart file and then read it into memory during the restart procedure. Writing and reading must be consistent.

Because tags, like `uO` and `ud`, are used in time history lists and plot lists to identify objects and lists, the user must ensure to use these tags. For example:

```
UserDefineList 'listName' {
  . . .
}
PlotList 'plotListName' {
  . . .
  udL-'listName' . . .
}
```

21.7.7 Time History Variables

This subsection explains how to create methods for extracting variables and printing them to a time-history list for user defined-lists and elements within a user-defined list. There are essentially five polymorphic methods that are used to accomplish this task.

```
int List::parseVariableIndex(string lbl, Reader *rdr);
Object *List::parseObject(Reader *rdr);
```

```
string List::makeVariableLabel(int elt, int var);
real List::getValue(int var);
real Object::getValue(int var);
```

The first two methods are used for reading the data from the input file. The last three methods are used for providing data labels and values to the methods that write to the time-history file. In the great majority of cases, the user wants to modify an existing class and implement a specific formulation. For this reason, we will explain the procedures using an example of a derived class.

Let's consider a new formulation for a tetrahedral element. This would rely on two classes: one for the tetrahedral element object, and the other one for the list of the new tets. These two classes are derived from the parent Tet class (for inheriting the geometrical properties and methods of a tetrahedral element) and ttLst class (for inheriting the methods of a tet list).

```
class Tet_UD : public Tet {
  . . .
};
class ttL_UD : public ttLst {
  . . .
};
```

Let's consider the case where we want to generate the time history of a parameter not currently available in the element formulation, for example the work perfomed by the internal forces. This quantity can be updated at each time step in the `calcFrc()` method and must be saved either as an additional state variable or as a new member of the class definition. If it is saved as an additional state variable, then it is easily accessed through the standard commands. Let's assume that we use a new member named t[wrk] which must explicitly appear in the class definition

```
class Tet_UD : public Tet {
  private:
     real wrk;  // new member
  . . .
};
```

The logical command in the input file for selecting the new quantity may look like this

```
TimeHistoryList Hist {
  . . .
  tt-'listName' 'elementIndex' InternalWork
}
```

where `InternalWork` is a keyword chosen to select the new member `wrk`. We also want to maintain the functionality already provided by the parent class. The way to accomplish this objective is to redefine the `parseVariableIndex()` method so that is assigns an

index of 1001 when it encounters the label `InternalWork`. Otherwise, it uses the method of the parent class. A large index is recommended so that it does not overlaps with smaller indices used in the parent class.

```
int ttL_UD::parseVariableIndex (string lbl, Reader *rdr) {
    if (lbl == "InternalWork")
        return 1001;
    else
        ttLst::parseVariableIndex(lbl, rdr);
}
```

Similarly, the user should redefine the method for generating the variable label in the time history file

```
string ttL_UD::makeVariableLabel (int elt, int var) {
    if (elt != 0 && var == 1001) {
        stringstream oss;
        oss << "ttL-" << name << "-" << elt << ":  internal work ";
        return (oss.str());
    } else
        return ttLst::makeVariableLabel(elt, var);
}
```

and the `getValue()` method in the user-defined element class

```
real Tet_UD:getValue (int var) {
    if (var == 1001)
        return wrk;
    else
        return Tet::getValue(var);
}
```

21.8 report a problem

If you are experiencing problems while setting up MARS input files and you are requesting help from ES3 staff, please use the following procedures for providing adequate information.

- Provide a brief description of the problem you are trying to solve and of the MARS model which you intend to use. The first two subsections of the problems described in the "MARS Example Library" document should give an idea of what would be useful, even though it is not necessary to go in great details. Figures of the geometry can be useful.
- Brief description of the difficulty encountered while setting up the input files or executing the simulation (screen captures can be useful)

- If possible, it would help if you can share the input files so that we at ES3 can do independent testing and debugging.

For clarity, organize the information in an e-mail in sections with section headings:

1. Problem Description
2. MARS Model and Input
3. Description of Encountered Difficulties
4. Input File Location (if applicable)

Realize that the more information you can provide, the easier it is for us to determine the problem and fix it or correct your input file.

22 Misc

22.1 Fluid Dynamic List

It is necessary to insert a fluid dynamic list when performing coupled calculations with fluid dynamic codes. The purpose of this list is to specify the entities that are used in the data exchange protocol. Only one fluid dynamic list can be specified and it requires no name. The contents of the list vary depending on which code MARS is coupled to. The 'FluidDynamicList' is typically entered at the bottom of the input file, possibly before the 'EOF' (End of File) line. The general syntax is

```
FluidDynamicList {
  . . .
}
```

Following are a list of codes to which MARS has been coupled to and the commands to specify the exchange data.

22.1.1 IFEM - (RPI)

The exchange protocol between MARS and IFEM establishes the following exchange of data. During the initialization phase MARS sends 1) the number of mesh nodes participating in the coupling, 2) their initial mass, and 3) their initial position. During the solution phase MARS receives 1) integration time step, which is controlled by IFEM, 2) velocities of the nodes and sends back 1) structural forces (internal and external) at the nodes.

Even if the selection defaults are chosen (all structural nodes and no facets) the 'FluidDynamicList' must be present in the input file. It this case, it is entered with no internal data like this:

```
FluidDynamicList {
}
```

A set of triangular faces from lists that had been previously defined can be selected and passed to IFEM during the initialization phase. phase.

```
  FluidDynamicList {
    tfL-'List1Name'}
    tfL-'List2Name'}
  }
```

22.1.2 Gemini

To be written

22.2 Mechanisms List

22.2.1 Shock Strut Assembly

The shock-strut assembly mechanism computes the forces generated by a shock absorber that connects two nodes in the model. At each step, the algorithm computes the distance between the nodes and their relative velocity in the direction aligned with them. The stroke is computed by subtracting the distance from a stroke offset input parameter:

```
Stoke = StrokeOffset - Distance
```

The value of the Stroke is used to interpolate a tabulated function ('ForceStrokeCurve'), which give the hydraulic static force generated by the gas or spring in compression. The range of the stroke is limited by maximum and minimum values. If the nodes try to move closer or further away then the stroke range allows, then they hit hard stops: these are implemented using penalty functions, with user-prescribed stiffness values. The viscous effect of hydraulic fluid is approximated using a linear expression:

```
DampingForce = Damping * RelativeVelocity
```

To avoid wild oscillations in the damping force, a moving average of the relative velocity is used:

$$V_{rel-movAv} = 0.99 * V_{rel-movAv} + 0.01 * V_{rel}$$

The two constants 0.99 and 0.01 are currently hard-coded. The input commands for the ShockStrut mechanism are given below:

```
Mechanisms {
  ShockStrut {
    FirstNode 'NodeListName' cl 0. cm 0. cm 10. cm
    SecondNode 'NodeListName' cl 0. cm 0. cm 40. cm
    ForceStrokeCurve 'CurveName'
    MinimumStroke 0. in
    MaximumStroke 16. in
    StrokeOffset  81. cm
    Stiffness 1.e6 lb/cm
    Damping 80000. N/m
  }
}
```

The units of damping are [Force]/[Velocity]. Since these units are currently not available in MARS, assume time is given in seconds and use units for [Force]/[Length].

The history of significant variables can be printed out using the following commands.

```
TimeHistoryList 'ListName' {
  . . .
  mm-'listName' Stroke
  mm-'listName' StaticForce
  mm-'listName' DampingForce
  mm-'listName' BottomTopForce
  mm-'listName' TotalForce
}
```

22.2.2 Brake

The brake mechanism provides a braking moment to a wheel. In this formulation the wheel motion is associated to that of a reference node; note that the wheel and tire can be modeled in great detail, however, it is necessary to associate a single node to the motion of the wheel and that node should be located on the axis of rotation. The formulation requires the definition of a 'Runway'; this is a flat surface which is identified by the first face of a face list. The face list can consist of triangular or quadrilateral faces. The surface is used to compute the distance of the axle from the surface and the direction of the axle parallel to the surface. The braking action is applied as a torque in the direction opposite of that of rotation. The time history of the braking action is prescribed using a load curve which is referenced using the 'BrakingHistory' command.

```
Mechanisms {
  Brakes {
    Node 'NodeListName' 'nodeIndex'
    Runway 'FaceListName'
    BrakingHistory 'CurveName'
  }
}
```

22.2.3 Anti-Lock Brake

The anti-lock brake mechanism . . .

```
Mechanisms {
  AntiLockBrakes {
    Node 'FrontWheels' 1
    Runway  'FaceList'
    RampUpRate ...
  }
}
```

22.3 Collection List

A 'collection list' is an assembly of lists that are grouped together for the purpose of performing the same operation on them. All these operations are done at the pre- or

post-processing phase. No actual computations are done during the solver loop. In the input block, the lists are first selected and then the operations on them are performed. Typical applications of this feature are:

```
1. Translate or rotate the entire model or part of it.
```

22.4 Unit Cell

The UnitCell class includes methods for generating a unit cell and for creating a list of constraints that enforce periodic conditions during a simulation of a unit cell. There are two phases: generation and simulation. The input for the generation phase has the following format: format:

```
Material Concrete RCConcrete Dev {
  MixDesign { . . . }
  StaticParameters { . . . }
}
UnitCell Cube {
  Material Concrete
  Side 2. in
  Seed 45435 // seed for random number generator
  Generate
}
```

The parameters for Material and Side are required, the seed is optional. The 'Generate' command forces MARS to write a mesh file for unit cell that has been generated. The mesh file is named 'UnitCellMesh.mrs'. Note that the nodes are periodic, but the tetrahedrals are not. This is because we have not been able to have tetgen generating periodic tet meshes, when the periodic external facets are prescribed.

The input for the solution phase has the following format:

```
Material Concrete RCConcrete Dev {
  MixDesign { . . . }
  StaticParameters { . . . }
}
TetSolidList UnitCell Ldpm {
  Material Concrete
  ReadFile UnitCellMesh.mrs
}
UnitCell Cube {
  Side 2. in
  TetList UnitCell
}
```

For the solution phase, the class 'UnitCell' creates a list of constraints that tie the nodes on the surface of the unit cell. Although the unit cell does not have a 'clean' geometric

shape, it is topologically similar to a cube.There are eight vertex nodes that are tied together. The vertex nodes can only rotate and their translations are set to zero. There are edge nodes that are grouped in sets of four; each set consists of four nodes on four parallel edges of the cube. There are face nodes that grouped in sets of two; each set consists of two nodes on opposite faces of the cube. The internal nodes do not appear in the constraints of the unit cell.

In the initialization phase, the masses of the nodes in each constraint are added up. The summed mass is then assigned to the nodes of the constraint. During execution, the forces and moments in each constraint are added up. The summed forces and moments are then assigned to the nodes of the constraint. This garantees that the nodes in the constraint move with the same velocity enforcing the conditions of periodicity.

22.5 Load Curve Lists

The LoadCurveList is used to defines a set of pressure time histories at certain spatial locations.

DYNA3D format

```
LoadCurveList BlastLoads {
  // 1.  Enter location and name of data file
  [ Directory  ../Loads/ ]
  Filename  pressures.dat
  Format dyna3D/shamrc/csv/mars
  // 2.  Enter spatial distribution type
  [ RefenceSystem  'RS name' ]
  Distribution Plane/Axisymmetric
  // 3.  Enter units
  X-Units time s
  Y-Units pressure psi
  Z-Units length in {1}
  // 4.  Enter curve mapping
  ReadObjects 'num-curves'
  // index     crx     cry
         1      5.      6.
  . . .
  // For axysymetric load
  ReadObjects 'num-curves'
  // index     rad
         1      0.
         2      1.
  . . .
  // 5.  Modify curves if necessary
  Y-Scale 5.
}
```

[1] The Z-Units are the location units in the table

SHAMRC files

This feature was inserted in Mars in 2004 in support of a study for assessing the effects of closed-in blast on suspension bridge cables. The pressure histories at selected locations on the surface of the cable were computed using the hydrocode SHAMRC. The pressure data was provided as a set of files, one file per station. In a separate table, each file was associated to the spatial coordinates of the station.

A SHAMRC LoadCurveList is typically used in conjunction with quadrilateral or triangular face lists. The mapping of load curve to face is generally done using the closest distance criterion. For more information, see the sections related to wet face lists.

```
LoadCurveList PRSS {
  fmt shamrc
  // 2. Enter location and name of data files
  dir cable04/TNT/run2/station
  num 624 // number of curves
  Read
  // for each curve enter
  //   1. index starting from 1
  //   2. label
  //   3. filename
  //   4. station coordinates
  1 C001 sta1.ovpr   10.0984  0  0
  2 C002 sta2.ovpr   9.33071  3.86614  0
  3 C003 sta2.ovpr   9.33071  -3.86614  0
  4 C004 sta3.ovpr   7.14173  7.14173  0
  5 C004 sta3.ovpr   7.14173  -7.14173  0
  . . .
  623 C623 sta331.ovpr   -9.33071  -3.86614  -190
  624 C624 sta332.ovpr   -10.0984  -0  -190
  cgs2psi
  X-Offset -9.54743E-04
}
```

Currently, Mars input variable are always defined with their dimensions. To satisfy this requirement, the input will be changed to the following format.

```
LoadCurveList PRSS {
  fmt shamrc
  // 2. Enter location and name of data files
  Folder cable04/TNT/run2/station
  NumberOfCurves 624 // number of curves
  TimeUnits s
  LengthUnits cm
```

```
  PressureUnits cgs
  ReadCurves
  // for each curve enter
  //   1. index starting from 1
  //   2. label
  //   3. filename
  //   4. station coordinates
  1 C001 sta1.ovpr   10.0984  0  0
  2 C002 sta2.ovpr   9.33071  3.86614  0
  3 C003 sta2.ovpr   9.33071  -3.86614  0
  4 C004 sta3.ovpr   7.14173  7.14173  0
  5 C004 sta3.ovpr   7.14173  -7.14173  0
  . . .
  623 C623 sta331.ovpr   -9.33071  -3.86614  -190
  624 C624 sta332.ovpr   -10.0984  -0  -190
  X-Offset -9.54743E-04 s
}
```

23 Computing Platforms

This section describes some of the specific set ups on the installation of Mars on specific computer centers. It is intended to help users setting up their computational environment on these platforms.

23.1 Mars on borg-SCOREC

The first time you use borg, you need to configure the system so that it can find Mars and MPI supporting software. Enter the bash shell:

```
> bash
```

Edit the .bashrc file in your main folder

```
$ vi ~/.bashrc
```

```
export PATH=.:/bigtmp/peless/Mars:/usr/local/openmpi64/latest/bin:$PATH
export LD_LIBRARY_PATH=$LD_LIBRARY_PATH:/usr/local/openmpi64/latest/lib
```

Insert the following two lines:Activate changes:

```
$ source ~/.bashrc
```

Any subsequent time you log in, start the bash shell and the path is automatically updated.

```
> bash
```

Interactive Execution

To run the OpenMP version of Mars, enter

```
$ mars0 input.mrs
```

To get the latest version of the built-in manual, enter

```
$ mars0 -H > manual
```

23.2 Mars on the CCNI system

The first time you use ccni, you need to configure the system so that it can find Mars and MPI supporting software. Enter the bash shell:

```
> bash
```

Edit the .bashrc file in your main folder:

```
$ vi ~/.bashrc
```

Insert the following line:

```
export PATH=.:/gpfs/small/MMCCpeld/Mars:/gpfs/small/MMCCpeld/bin:$PATH
```

The `MMCCpeld/bin` folder contains auxillary codes like `tetgen` that may be used for specific tasks, such as model generation of LDPM tetrahedral meshes. Activate changes:

```
$ source ~/.bashrc
```

Any subsequent time you log in, start the bash shell and the path is automatically updated.

```
> bash
```

Interactive Execution

To run the OpenMP version of Mars, enter

```
$ mars0 input.mrs
```

To get the latest version of the built-in LaTex manual, enter

```
$ mars0 -Dl
```

Batch Execution

To run the OpenMP version of Mars in batch mode, create a script (e.g. `job.sh`)

```
#!/bin/bash
echo 'job starting'
cd 'yourProblemFolder'
mars0 -B input.mrs > output
```

Then submit it using the sbatch command:

```
   sbatch -p opterons -n 1 -t 120 -o ./out ./job.sh
where
  -p opteron: is the partition
  -n 1: is the number of compute nodes
  -t 120: is the maximum time in minutes
  -o ./out: is where the output goes
  job.sh: is the input script
```

To check status, type `squeue`. To list partitions, type `sinfo`

Batch Execution - MPI

First, you must configure your envirnoment. Information can be found at

`wiki.ccni.rpi.edu/index.php/RedHat_5_and_Modules]`

Load the MPI environment:

```
module load mpi/openmpi-1.4-gcc41
```

Create a script file (e.g. `job.sh`) to control batch execution

```
#!/bin/bash
echo 'job starting'
cd 'yourProblemFolder'
mpirun -n 32 marsM -B input.mrs > output
```

Then submit it using the sbatch command:

```
sbatch -p opterons -n 32 -t 120 -o ./out ./job.sh
```

23.3 Mars on NWU Quest

The first time you use quest, you need to configure the system so that it can find Mars and MPI supporting software. Enter the bash shell:

```
> bash
```

Edit the .bashrc file in your main folder:

```
$ vi ~/.bashrc
```

Insert the following line:

```
export PATH=.:/hpc/home/dpw466/Mars:$PATH
```

```
$ source ~/.bashrc
```

Any subsequent time you log in, start the bash shell and the path is automatically updated.

```
> bash
```

Interactive Execution

To run the OpenMP version of Mars, enter

```
$ marsO input.mrs
```

To get the latest version of the built-in LaTex manual, enter

```
$ marsO -Dl
```

Batch Execution - MPI

Load the MPI environment:

```
module load mpi/openmpi-1.4.3-gnu
```

Create a script file (e.g. `job.sh`) to control batch execution

```
#!/bin/bash
#MOAB -l nodes=4:ppn=8
#MOAB -l walltime=0:59:00
#MOAB -j oe
#MSUB -A p20288
ulimit -s unlimited
cd 'yourProblemFolder'
mpirun marsM -B input.mrs > output
```

Then submit it using the sbatch command:

```
msub job.sh
```

Check the status using the command:

```
showq | grep x
```

where `x` is your username.

23.4 Mars on hpc-diamond

Diamond contains 1,920 compute nodes (15,360 compute cores). Each compute node contains two 2.8-GHz Intel Xeon 64-bit quad-core Nehalem processors and 24 GBytes of dedicated memory. The nodes are connected to each other in a HyperCube topology DDR 4X InfiniBand network.

Pre-Processing

The Intel c++ compiler (`icc`) is available on diamond and this is the software that should be use for pre-processing a Mars input file. The syntax is

```
icc -E -D... input.mrs > inputP.mrs
```

Executing the OpenMP version of Mars

The OpenMP versions of Mars are stored in the `/usr/local/u/peless/Mars/` folder. Executables are named using the following convention, `marsO-yymmdd` or `marsOyymmdd`, where `yymmdd` is a six digit number representing the date of the executable. `marsOyymmdd` employs the shared memory model. On diamond it can only be executed on a single compute node over 8 compute cores. A typical bash script is listed below

```
#!/bin/bash
#PBS -A ERDCV02221SPS
#PBS -l walltime=10:00:00
#PBS -N Ldpm4pt2
#PBS -q standard
#PBS -j oe
#PBS -l select=1:ncpus=8:mpiprocs=1
# select = compute nodes requested
# ncpus must equal 8
# mpiprocs = cores/node
#PBS -l place=scatter:excl
# Allows PBS to use any available nodes. Excludes other users
# from using your nodes while they are scheduled to you
cd /work/peless/1104Jov/4pt2
export OMP_NUM_THREADS=8
/usr/local/u/peless/Mars/marsO110524 -B input.mrs > outOMP

# if you are using the C shell
setenv OMP_NUM_THREADS 8
/usr/local/u/peless/Mars/marsO110524 -B input.mrs
```

Executing the MPI version of Mars

The MPI versions of Mars are stored in the `/usr/local/u/peless/Mars/` folder. Executables are named using the following convention `marsM-yymmdd` or `marsMyymmdd`, where

yymmdd is a six digit number representing the date of the executable. marsM employs the distributed memory model. On diamond it can only be executed on multiple compute nodes and offers much bigger performance gains over the OpenMP version. A typical script is shown below

```
#!/bin/bash
#PBS -A ERDCV02221SPS
#PBS -l walltime=10:00:00
#PBS -N Ldpm4pt2
#PBS -q standard
#PBS -j oe
#PBS -l select=4:ncpus=8:mpiprocs=8
# select = compute nodes requested
# ncpus must equal 8
# mpiprocs = cores/node
#PBS -l place=scatter:excl
# Allows PBS to use any available nodes. Excludes other users
# from using your nodes while they are scheduled to you
cd /work/peless/1104Jov/4pt2
mpiexec_mpt -np 32 /usr/local/u/peless/Mars/marsM110524 -B input.mrs > out032
```

Executing the Hybrid version of Mars

Since 2009, the marsM version of mars implements the hybrid model. In a 'hybrid' execution, multiple instances of the code are run on multiple compute nodes and each instance runs multiple OpenMP threads. For example, one can run 16 instances and each instance runs four threads. This requires 16x4 = 64 compute cores = 8 compute nodes. The commands for executing this hybrid run are

```
# if you are using the C shell
setenv OMP_NUM_THREADS 4
mpirun -np 16 /usr/local/u/peless/Mars/marsM110524 -B input.mrs
```

It appears that there is a slight benefit in running the hybrid version up to 4 threads. When 8 threads are used, there is no significant benefit. This may be because as long as a processor is using its 4 cores on 4 parallel threads, the four threads work very efficiently. When 8 threads are run on two processors, then there may be conflicts in accessing the shared memory. In any case, testing on a specific problem may be the best way to figure out the optimal configuration.

```
#!/bin/bash
#PBS -A ERDCV02221SPS
#PBS -l walltime=10:00:00
#PBS -N Ldpm4pt2
#PBS -q standard
#PBS -j oe
```

```
#PBS -l select=4:ncpus=8:mpiprocs=2
# select = compute nodes requested
# ncpus must equal 8
# mpiprocs = cores/node
#PBS -l place=scatter:excl
# Allows PBS to use any available nodes. Excludes other users
# from using your nodes while they are scheduled to you
cd /work/peless/1104Jov/4pt2
export OMP_NUM_THREADS=4
mpiexec_mpt -np 8 /usr/local/u/peless/Mars/marsM110524 -B input.mrs > out032
```

23.5 Mars on Windows PCs

PC versions of MARS are also available for computers using the MS Windows operating system. However, since most of the development and execution of MARS is done on Unix based computers (including Apple computers which employ a Unix based operating systems), we recommend that the Windows PC intended for usage has the cygwin software installed. As most of engineers already know, cygwin provides a Unix like interface to PC users. The following directives are given assuming that cygwin is available. This approach makes it possible to use MARS consistently across different operating systems.

Note that the default installation of cygwin does not provide all the functionality that is needed. You must check additional modules.

This is compiled using the Visual Studio 2008 C++ compiler.

First, place the executable `marsW` in a folder of your choice and either put that folder in the `PATH` or make an alias

```
alias mars=$MARSPATH/marsWvs
```

so that marsWvs is executed when you type `mars` at the prompt. Try it typing `mars -h` to start an interactive help session and enter `Q` to exit).

24 Pre-Processing and Mesh Generation Software

Mars interfaces with two mesh generation packages for creating tetrahedral solid meshes (tetgen) and two-dimensional triangular meshes (Triangle). Both programs are freely available to researchers on the Internet. Both programs are copyrighted. To avoid copyright infringment, ES3 is not distributing source or binaries for the two programs, but we are refering users to download software from their respective websites and install them following the directions provided by the authors.

Both programs are executed as external modules. More precisely, MARS writes input files for either program, executes the programs as separate threads using the `command()` function, and reads the mesh from the output files created by the programs. This process is transparent to the user. However, it is critical to have the two programs available in the `PATH`. This can be accomplished in two ways. First, symbolic links can be created in a folder already in the `PATH` that point to the executables:

```
ln -s $TETGEN-FOLDER/tetgen $BIN-FOLDER/tetgen
```

Second, the folders where the executable have been generated can be placed in the `PATH`:

```
export PATH=$PATH:$TETGEN-FOLDER:$TRIANGLE-FOLDER
```

Note: in the lines above, `$TEGEN-FOLDER`, `$TRIANGLE-FOLDER`, and `$BIN-FOLDER` must be replaced by the names of actual folders.

24.1 Triangle

Triangle generates exact Delaunay triangulations, constrained Delaunay triangulations, conforming Delaunay triangulations, Voronoi diagrams, and high-quality triangular meshes. The latter can be generated with no small or large angles, and are thus suitable for finite element analysis.

Triangle was developed by Dr. Jonathan R. Shewchuck and is available at

```
http://www.cs.cmu.edu/~quake/triangle.html
```

Triangle is used in Mars for generating triangular meshes of flat surfaces.

24.2 Tetgen

TetGen is a program to generate tetrahedral meshes of any 3D polyhedral domains. TetGen generates exact constrained Delaunay tetrahedralizations, boundary conforming Delaunay meshes, and Voronoi partitions.

Triangle was developed by Dr. Hang Si and is available at

```
http://wias-berlin.de/software/tetgen/
```

Tetgen is used in Mars mainly for generating tetrahedral meshes for LDPM models.

25 Post-Processing Software

25.1 Quasar

QUASAR is the graphical postprocessor for the MARS results.

There are two version of the QUASAR program. The first version is based on the GLUT library The second version is written in JAVA

Both versions have been ported to various operating systems. The JAVA version is no longer supported.

25.1.1 Quasar User Manual (GLUT)

The version of QUASAR is written in C++. It employs OpenGL for 3-D rendering and GLUT for a rudimentary UI. It requires the user to memorize the functionality of some of the keyboard keys but it is a lot faster than the Java version for rendering large models. It had been tested under Linux and under Windows (cygwin).

Viewing plot files using QUASAR

The plot files generated by Mars are viewable using the quasar post-processor. quasar is based on the OpenGL library for three-dimensional rendering. The execution command is

```
quasar [input file name]
```

Currently, quasar does not have a fully developed GUI interface, although it uses the pop-up menus provided by the GLUT library for many of its tasks. To make thinks efficient, control of the model is done by a combination of keyboard hits and mouse motion.

Repositioning the model

The model can be repositioned by rotating, translating, and zooming the model in front of the viewer. The motion is achieved by moving the mouse. In earlier versions of Quasar, the functionality of the mouse motions was preselected by pressing one of these four keys 't', 'r', 'e', and 'w'.

t: turn translation on

r: turn rotation around two axis on

e: turn zooming on (motion of the mouse up and down)

w: turn spinning in the third direction on (motion of the mouse left and right)

When manipulating the model, (if you are right handed) you would keep the four fingers of the left hand on the w, e, r, and t keys and the right hand on the mouse. You can then click the key to select what motion the mouse affects and move the model using the mouse.

In later versions of Quasar, the functionality was modified to be consistent with the functionaly of Paraview.

Simple click and drag: turn model around the two axis co-planar with the screen

Click and drag while pressing the [Shift] key: spin model around axix perpendicular to the screen.

Click and drag while pressing the [Control] key: zoom in and out

Click and drag while pressing both the [Shift] and [Control] keys simultaneously: translate the model. [Mar 2011] The combination [Shift] [Control] does not work on Windows/Cygwin, quasar was slightly modified so that translation can also be accomplished by pressing the [Alt] key on all systems.

Advancing frames in a family of files

If mars had generated a family of files during its execution,(for example, a series of `PLOT.000, PLOT.001, PLOT.002` files created by the `PlotList PLOT` command) you can move back and forth through the sequence pressing the < and > keys. If your graphics card is fast enough and the model is not too complicated you can achieve a good animation effect interactively.

Saving and loading a viewing configuration

If you like the way the model is being displayed, you can save the configuration parameters by pressing the [Shift]W (write) key. At any time the model can be redisplayed in the saved configuration by pressing the [Shift]R (read) key.

Viewing mesh grids, outlines, faces and particles.

When quasar starts, the outline, faces, and particles are automatically displayed. It is possible to toggle all these quantities on and off by pressing the 'f', 'g', 'o', and 'p' keys:

f: toggle displaying of all faces in the model
g: toggle displaying of the mesh grid
o: toggle displaying of outline
p: toggle displaying of spherical particles (and cylindrical surfaces)

This can be very useful when dealing with a complex model where it takes a while to repaint the frame. In such cases, particles and faces can be turned off and the model can be repositioned quickly using its outline. Once the desired position is achieved, toggle on the desired entities.

Saving the screen to a graphics file

You can save the current quasar screen to a ppm file that can be later incorporated in a WORD document by pressing the [Shift]-G key. This generates a file named ..

Turning model components on and off

You can select what parts of the models to display by pressing the right button of the mouse. This action brings a pop-up menu with six entries. Select [Model] and the rest should be intuitive.

Making frames for an animation

Press [Shift]M (movie) or press the right button of the mouse to bring up the pop-up menu and select [Options][Generate Movie Frames]. This will generate a sequence of plot.ppm.nnn files that can be later linked to make a Quicktime movie file.

25.1.2 Quasar File Format

The ASCII format for QUASAR input files consists of a set of optional information lines and a set of geometric entity lists. Currently, QUASAR is able to render five types of geometric entities:

1. Spheres
2. Lines
3. Cylinders

4. Triangular faces

5. Quadrilateral faces

A sample input file is given at the bottom of this page.

Spherical Entities

QUASAR renders spherical entities in the model using multi-faceted solids. Three different resolutions are available. The lower resolution, which is the default, is suitable for very large models. Medium and high resolutions generate smoother spheres but require more system resources and may take several seconds for each update. The resolution can be set in the input file with an optional command line or changed interactively for each list during execution via pop-up menu. The spheres are painted in light gray unless a specific color is selected using the `color` command line. Sphere data is entered one line per sphere. The first field is the sphere index followed by the three coordinates and the radius. The sphere index does not have to be in sequence. Thus, if a subset of a longer list is used, the original indeces can be used. If the user wants to scale the spheres after the file has been created, this can be accomplished using the optional `scale` command line.

```
npL LABL
  [ color clr ]
  [ resolution high / medium / low ]
  [ scale s ]
  numnp n
  crd
    i1 x1 y1 z1 r1
    i2 x2 y2 z2 r2
    . . .
    in xn yn zn rn
  eoL
}
```

The spheres can be painted colors continuously varying from blue to red to create `fringe` plots of physical quantities. To exercise this option, the fringe command line must be present before the sphere data is entered, as shown in the example below. The fringe keyword is followed by the range for the scalar variable to be used for painting. For each particle, the scalar variable follows the radius.

```
npL LABL
  fringe fmin fmax
  [ resolution (high, medium, low) ]
  [ scale s ]
  numnp n
  crd
```

```
    i1 x1 y1 z1 r1 f1
    i2 x2 y2 z2 r2 f2
    . . .
    in xn yn zn rn fn
  eoL
```

Lines

Line lists are used for a variety of purposes. For example, they can be used to outline the sharp edges of a solid part or the edges of shell parts. They also can be used to trace the axis of beam elements for quick rendering, short segments perpendicular to triangular or quadrilateral faces to indicate positive directions. Lines are typically painted with a uniform solid color defined by the keyword `color`. The default color is black.

```
eeL LABL
  [ color color ]
  numpt n
  crd
    i1 x1 y1 z1
    i2 x2 y2 z2
    . . .
    in xn yn zn
  numee m
  list
    i1 j11 j12
    i2 j21 j22
    . . .
    im jm1 jm2
  eoL
```

It is also possible to paint lines with colors that vary continuously from blue to red to create fringe plots of physical quantities. To exercise this option, the `fringe` command line must be entered after the list block, as shown in the example below. The `fringe` keyword is followed by the range for the scalar variable to be used for painting.

```
eeL LABL
  [ color color ]
  numpt n
  crd
    i1 x1 y1 z1
    i2 x2 y2 z2
    . . .
    in xn yn zn
  numee m
  list
    i1 j11 j12
```

```
    i2 j21 j22
    . . .
    im jm1 jm2
  fringe fmin fmax
    f11 f12
    f21 f22
    . . .
    fm1 fm2
  eoL
```

Cylinders

The reason for this type of list is for representing cylindrical surfaces of structural members such as wires, cables, rebars etc. Figure 1 shows a section of a 7x7 twisted cable consisting of 49 wires. The left picture shows a wireframe representation, while the right picture shows a solid rendering of the wires using cylindrical surfaces. It is obvious why the solid representation is superior. The format and amount of data in the plot files for the two types of lists is essentially the same. The `csL` lists have two extra parameters: `radius` and `resolution`.

```
csL LABL
  [ front color ]
  radius r
  [ resolution low / medium / high ]
  numpt n
  crd
    i1 x1 y1 z1
    i2 x2 y2 z2
    . . .
    in xn yn zn
  numcs m
  list
    i1 j11 j12
    i2 j21 j22
    . . .
    im jm1 jm2
  eoL
```

It is also possible to paint cylindrical setctions with colors that vary continuously from blue to red to create fringe plots of physical quantities. To exercise this option, the fringe command line must be entered after the list block, as shown in the example below. The `fringe` keyword is followed by the range for the scalar variable to be used for painting.

```
csL LABL
  numpt n
  crd
```

```
    i1 x1 y1 z1
    i2 x2 y2 z2
    . . .
    in xn yn zn
  numcs m
  list
    i1 j11 j12
    i2 j21 j22
    . . .
    im jm1 jm2
  [ smooth ]
  fringe fmin fmax
    f11 f12
    f21 f22
    . . .
    fm1 fm2
  eoL
```

Triangular Faces

Triangular face lists are used for rendering surfaces consisting of triangular faces. These may be generated from triangular shell meshes or external faces of tetrahedral meshes.

```
tfL LABL
  [ front color ]
  [ back color ]
  numpt n
  crd
    i1 x1 y1 z1
    i2 x2 y2 z2
    . . .
    in xn yn zn
  numtf m
    i1 j11 j12 j13
    i2 j21 j22 j23
    . . .
    im jm1 jm2 jm3
eoL
```

Contour and fringe plots are possible

```
tfL LABL
  numpt n
  crd
    i1 x1 y1 z1
    i2 x2 y2 z2
```

```
    . . .
    in xn yn zn
  numtf m
    i1 j11 j12 j13
    i2 j21 j22 j23
    . . .
    im jm1 jm2 jm3
  [ smooth ]
  fringe fmin fmax
    f11 f12 f13
    f21 f22 f23
    . . .
    fm1 fm2 fm3
  eoL
```

Quadrilateral Faces

Quadrilateral face lists are used for rendering surfaces consisting of quadrilateral faces. These may be generated from quadrilateral shell meshes or external faces of hexahedral meshes.

```
qfL LABL
  [ front color ]
  [ back color ]
  numpt n
  crd
    i1 x1 y1 z1
    i2 x2 y2 z2
    . . .
    in xn yn zn
  numqf m
    i1 j11 j12 j13 j14
    i2 j21 j22 j23 j24
    . . .
    im jm1 jm2 jm3 jm4
eoL
```

Contour and fringe plots are possible

```
qfL LABL
  numpt n
  crd
    i1 x1 y1 z1
    i2 x2 y2 z2
    . . .
    in xn yn zn
```

```
  numqf m
    i1 j11 j12 j13 j14
    i2 j21 j22 j23 j24
    . . .
    im jm1 jm2 jm3 jm4
  [ smooth ]
  fringe fmin fmax
    f11 f12 f13 f14
    f21 f22 f23 f24
    . . .
    fm1 fm2 fm3 fm4
  eoL
```

Example

In this complete listing of an acutal file, note that the first three lines are used for reference information that can be printed when displaying the image. The words `title`, `steps`, and `time` are keywords.

```
title DPM grid and associated tet mesh
nsteps 0
time 0.000000
tfL NAME
  front lightgray
  back null
  numpt 995
  crd
      1      -1.200       0.000       6.800
      2      -1.200       0.000       7.100
      3      -1.200       0.000       7.400
      4      -1.200       0.000       7.700
   . . .
   2548       1.200       6.000       7.800
   2549       1.200       6.000       8.000
  numtf 1988
  list
    1     1   151   147
    2   148     1   147
    3     2     7     1
. . .
 1987   995   761   835
 1988   761   995   850
  eoL
eeL NAME
  color black
```

```
  numpt 207
  crd
      1      -1.200       0.000       6.800
      2      -1.200       0.000       7.100
   . . .
   2549       1.200       6.000       8.000
  numee 218
  list
     1     2     1
     2     1     6
   . . .
   217   205   206
   218   206   207
  eoL
npL GRID
  color lightgray
  numnp 1064
  crd
      1       0.506       2.563       7.720       0.200
      2      -0.055       1.495       7.545       0.200
      3       0.291       4.280       5.850       0.200
      4      -0.827       1.526       7.474       0.200
   . . .
   1063       0.059       4.546       4.857       0.100
   1064      -0.375       3.228       5.850       0.100
  eoL
EOF
```

25.2 jHist: a java post-processor for Mars time history files

`jHist` is a rather simple java program for quickly displaying time histories generated by Mars using the TimeHistoryList commands. `jHist` defaults the x-axis to the first record in the time history file (which is typically the time in milliseconds) and the y-axis to the second record. After the initial plot is displayed, the records for the x- and y-axis can easily be changed to any other record in the file using the scroll-down menu options. It is possible to display multiple curves simultaneously. At the moment, all curves are plotted using a continuous thin solid black line.

25.2.1 Installation

`jHist` requires the Java Runtime Environment (JRE) to be installed on your computer. You can quickly check if JRE is installed by typing:

```
  $ which java
```

If JRE is not installed, google 'installing java' and choose one of the www.java.com sites. Installing JRE is free and simple.

The java class files for jHist are typically placed in a folder named `$MARSPATH/jHist`, where `MARSPATH` is an environment variable that contains the path of the folder where Mars files are located. The best way to incorporate jHist is to insert the defintion of `MARSPATH` and an alias in your .bashrc file

```
export MARSPATH=/.../.../Mars  # replace ... with actual path
alias jHist="java -cp $MARSPATH/jHist jHist"
```

For PC-cygwin users, it is important to type the correct path (the Windows path, rather than the cygwin path), e.g.:

```
alias jHist="java -cp c:/cygwin/home/$USER/Mars/jHist jHist"
```

Note that a java program consists of a series of files with the `.class` extension. These files are executed through the JRE and are OS independent. Thus, they can be installed on any computer.

25.2.2 Execution

If the alias for `jHist` is properly set, then, the plots for file `Hist.th` can be executed from the folder where the file is located using the command:

```
jHist Hist
```

We have not been able to execute `jHist` (and `jCurv`) over a `ssh` session, even when other X11 applications could be executed. This would be a very desirable capability, since it would eliminate the need to download history files from a supercomputer center to you local computer. Unlike 3-D graphical applications that can be executed but are too slow to be practical, `jHist` could be run very effectively from a remote server. If anybody can figure out how to do this, please let's us know, and we will make this feature available to everybody else.

25.2.3 File format

Time history files have the following structure:

```
1: title line
2: number of records  (n)
3.1: label for first record
3.2: label for second record
. . .
3.n: label for nth record
4.0:  v_0,1  v_0,2  . . .  v_0,n   values at time v_0,1 (typically 0.)
4.1:  v_1,1  v_1,2  . . .  v_1,n   values at time v_1,1
. . .
4.m:  v_m,1  v_m,2  . . .  v_m,n  values at time v_m,1
```

The labels in section 3 of the input are used in the drop down menus for selecting the records to be displayed.

25.3 jCurv: a java program for making plots from various source files

jCurv is a simple utility for creating plots of multiple curves from different source files. jCurv is also written in Java. It is a batch program with the plot formatting commands entered in an ASCII file. jCurv generates plot images that can be saved to png files for incorporation in documents. Its execution is very simple. At the command line, enter

```
$ jCurv 'filename'
```

where 'filename' is the name of the input file without the required extension .jcr. For example, if the input filename is compare.jcr, the command would be jCurv compare.

jCurv creates a 3 in by 5 in plot and two actions are available. The Refresh button makes it possible to refresh the plot when one or more of the source files are continuosly updated during an ongoing simulation. The Make .png button makes it possible to save the image to file image.png in the local folder. If you need to generate mulitple files, you have to change the name to avoid overwriting previous images.

Installation is similar to jHist. You need to include an alias entry in the .bashrc file, similarly to what was done for jHist. The jCurv classes are typicall installed in the $MARSPATH/jCurv folder. Some examples are also included. They are named example1.jcr, example2.jcr, etc.; the data sets used in the examples are named dataset1.th, dataset2.th, etc.

25.3.1 Input file format

The format of the input file is discussed by explaining the commands contained in example1.jcr (one of the examples included in the installation):

```
 1: Title  Example
 2: XAxis lb "X-Axis" mn 0. dl 0.1 fm 0.0  L 4
 3: YAxis lb "Y-Axis" mn -2. dl 2. fm 0.
 4: Load DS1 mars dataset1.th
 5: Band  xr DS1 1  ybr DS1 2  ytr DS1 3  fill
 6: Band  xr DS1 1  ybr DS1 2  ytr DS1 3  cl black
 7: Load DS2 seq dataset2.th
 9: Curve  xr DS2 1  yr DS2 3  cl green
 8: Curve  xr DS2 1  yr DS2 2  cl blue  triangles
10: Load DS3 xy dataset3.th
11: Curve  xr DS3 1  yr DS3 2  xs 0.1  cl red
12: EOF
```

Although the sequence of commands can be changed, the order may affect the final look of the plot. Following is an explanation of the various lines.

Line 1: the title line is not used in the plot, but can be used as a comment line.

Line 2: the second line specifies the format of the x-axis using the following arguments: lb Title of the x-axis; mn value of the first tic; dl increment for each tic; fm format for

tic value, number of zeros after period corresponds to the number of decimal digits. The default length of the x-axis is five inches, which major tick at one inch intervals.

Line 3: the second line specifies the format of the y-axis using the following arguments: `lb` Title of the y-axis; `mn` value of the first tic; `dl` increment for each tic; `fm` format for tic value, number of zeros after period corresponds to the number of decimal digits. The default length of the x-axis is three inches, which major tick at one inch intervals. It is possible to make the height two inches long using the `L 2` command.

Line 4: The `Load` command is used to load a data set in memory. A data set consists of a set of two or more records, represented as arrays of real numbers. The label `DS1` is a token to be used to identify the load set in following lines; `mars` is a keyword to identify the format of the data-file; `dataset1.th` is the name of the data-file. Two additional file formats are available: `seq` at line 7 and `xy` at line 11. Both formats are explained below.

Line 5: The `Band` command is used to depict an area limited by an upper and a lower curve. Two types of bands are available: 1) a solid band where the area is filled with a lightgray color, 2) a striped band consisting of vertical lines connecting lower and upper curves at the given data points. The arguments of the command are: `xr DS1 1` means use record number 1 from the `DS1` dataset for the x-axis value, `ybr DS1 2` means use record number 2 for the lower y value, `ytr DS1 3` means use record number 3 for upper y values, `fill` means paint the band using a solid color rather than vertical lines.

Line 6: This command is similar to the command in line 5, but represents the band using vertical lines in black color.

Line 8: The `Curve` command is used draw lines or symbols to visualize time history data or experimental data-points. The arguments of the command are: `xr DS2 1` means use record number 1 from the `DS2` dataset for the x-axis; `yr DS2 3` means use record number 3 from the `DS2` dataset for the y-axis; `cl green` means paint the line in green, the following colors are available: black, blue, red, green, cyan, yellow, magenta, orange, gray, and lightgray (the default color is black).

Line 11: In this line, the command `xs 0.1` means that the x-coordinates are multiplied (scale) by the 0.1 factor. Three other similar commands are available for both `Band` and `Curve` commands: `xo offset`, `ys scale`, and `yo offset`. These are used to scale and offset the original records using the equation:

```
new_value = scale*old_value + offset
```

Line 12: The `EOF` line terminates the input phase, any information after the EOF line is ignored.

This is the sequence in which the various plot elements are displayed: first, the solid bands, if any, are painted in light gray. Then, the x- and y-axis, and grid are painted in various shades of gray or black. Then, the curves or symbols are painted, and finally the vertical bands.

25.3.2 Data set file formats

`jCurv` accepts the file format of the time history files generated by Mars from the `TimeHistoryList's`. Furthermore, it accepts two other file formats. Data which may

be available in ASCII format can be edited to satisfy one of the three formats using an ASCII editor. If you have a specific format which you would like to be incorporated, please make a request to ES3. All files formats are included in the examples.

Format of 'xy' files

```
x_1 y_1
x_2 y_2
. . .
x_n y_n
```

Format of 'seq' files

```
Title line          // (string)
Title line          // (string)
nRec                // (int) number of Records
Record-1-label      // (string)
npt                 // (int) number of value for record 1
value-1-1           // first value of record 1
value-1-2           // second value of record 1
. . .
value-1-npt         // npt-th value of record 1
Record-2-label      // (string)
npt                 // (int) number of value for record 2
value-2-1           // first value of record 2
value-2-2           // second value of record 2
. . .
value-2-npt         // npt-th value of record 2
. . .
. . .
Record-nRec-label   // (string)
npt                 // (int) number of value for record nRec
value-nRec-1        // first value of record nRec
value-nRec-2        // second value of record nRec
. . .
value-nRec-npt      // npt-th value of record nRec
```